# Identifiability of Graphs with Small Color Classes by the Weisfeiler-Leman Algorithm

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#### Abstract

As it is well known, the isomorphism problem for vertex-colored graphs with color multiplicity at most 3 is solvable by the classical 2-dimensional Weisfeiler-Leman algorithm (2-WL). On the other hand, the prominent Cai-Fürer-Immerman construction shows that even the multidimensional version of the algorithm does not suffice for graphs with color multiplicity 4. We give an efficient decision procedure that, given a graph G of color multiplicity 4, recognizes whether or not G is identifiable by 2-WL, that is, whether or not 2-WL distinguishes G from any non-isomorphic graph. In fact, we solve the much more general problem of recognizing whether or not a given coherent configuration of maximum fiber size 4 is separable. This extends our recognition algorithm to graphs of color multiplicity 4 with directed and colored edges.

Our decision procedure is based on an explicit description of the class of graphs with color multiplicity 4 that are *not* identifiable by 2-WL. The Cai-Fürer-Immerman graphs of color multiplicity 4 distinctly appear here as a natural subclass, which demonstrates that the Cai-Fürer-Immerman construction is not ad hoc. Our classification reveals also other types of graphs that are hard for 2-WL. One of them arises from patterns known as  $(n_3)$ -configurations in incidence geometry.

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# 1 Introduction

Over 50 years ago Weisfeiler and Leman [36] described a natural combinatorial procedure that since then constantly plays a significant role in the research on the graph isomorphism problem. The procedure is now most often referred to as the 2-dimensional Weisfeiler-Leman algorithm (2-WL). It generalizes and improves the classical color refinement method (1-WL) and has an even more powerful k-dimensional version (k-WL) for any k > 2. The original 2-dimensional version

and the logarithmic-dimensional enhancement are important components in Babai's quasipolynomial-time isomorphism algorithm [4].

Even on its own, 2-WL is a quite powerful tool in isomorphism testing. For instance, it solves the isomorphism problem for several important graph classes, in particular, for interval graphs [16]. Also, it is successful for almost all regular graphs of a fixed degree [5]. On the other hand, not every pair of non-isomorphic graphs is distinguishable by 2-WL. For example, it cannot detect any difference between two non-isomorphic strongly regular graphs with the same parameters.

We call a graph G amenable to k-WL if the algorithm distinguishes G from any non-isomorphic graph. An efficient characterization of the class of graphs amenable to 1-WL is obtained by Arvind et al. in [2], where it is given also for vertex-colored graphs. Independently, Kiefer et al. [26] give an efficient criterion of amenability to 1-WL in a more general framework including also directed graphs with colored edges. Similar results for 2-WL are currently out of reach, even for undirected uncolored graphs. A stumbling block here is the lack of understanding which strongly regular graphs are uniquely determined by their parameters. Note that a strongly regular graph is determined by its parameters up to isomorphism if and only if it is amenable to 2-WL.

A general strategy to approach a hard problem is to examine its complexity in the parameterized setting. We consider vertex-colored graphs with the color multiplicity, that is, the maximum number of equally colored vertices, as parameter. If this parameter is bounded, the graph isomorphism problem is known to be efficiently solvable. More specifically, it is solvable in time polynomial in the number of vertices and quasipolynomial in the color multiplicity [4, Corollary 4], and it is solvable in polylogarithmic parallel time [29]. Graph Isomorphism is known to be in the  $\text{Mod}_k L$  hierarchy for any fixed color multiplicity [3], and even in the class  $\oplus L = \text{Mod}_2 L$  for color multiplicity 4 and 5; see [1]. Recall that  $\text{Mod}_k L$  is the class of decision problems solvable non-deterministically in logspace in the sense that the answer is "no" if and only if the number of accepting paths is divisible by k.

Every graph of color multiplicity at most 3 is amenable to 2-WL (Immerman and Lander [25]). Starting from the color multiplicity 4, the amenability concept is non-trivial: The prominent Cai-Fürer-Immerman construction [9] shows that for any k, there exist graphs with color multiplicity 4 that are not amenable to k-WL.

We design an efficient decision procedure that, given a graph G with color multiplicity 4, recognizes whether or not G is amenable to 2-WL. Note that an a priori upper complexity bound for this decision problem is coNP, as a consequence of the aforementioned fact that Graph Isomorphism for graphs of bounded color multiplicity is in P. From now on, amenability is meant with respect to 2-WL, unless stated otherwise.

We actually solve a much more general problem. 2-WL transforms an input graph G, possibly with colored vertices and directed and colored edges, into a *coherent* configuration C(G), which is called the *coherent closure* of G. The concept of a coherent configuration has been discovered independently in statistics [6] and algebra [21] and, playing an important role in diverse areas, has been developed to the

subject of a rich theory; see a recent monograph [10], that we will use in this paper as a reference book. A coherent configuration  $\mathcal{C}$  is called *separable* if the isomorphism type of  $\mathcal{C}$  is determined by its regularity parameters in a certain strong sense; see the definition in Section 2. The separability of the coherent closure  $\mathcal{C}(G)$  implies the amenability of the graph G. This was the approach undertaken in [16], where it was shown that the coherent closure of any interval graph is separable. Somewhat less obviously, the converse relation between amenability of G and separability of  $\mathcal{C}(G)$  is also true: For every graph G,

$$G$$
 is amenable if and only if  $\mathcal{C}(G)$  is separable; (1)

see Theorem 2.5 in Section 2. Equivalence (1) reduces the amenability problem for graphs to the separability problem for coherent configurations. This reduction works as well for directed graphs with colored vertices and colored edges, that is, essentially for general binary relational structures. If G has color multiplicity b, then the maximum fiber size of  $\mathcal{C}(G)$  is also bounded by b. While all coherent configurations with fibers of size at most 3 are known to be separable [10], the separability property for coherent configurations with fibers of size 4 is non-trivial, and our first result is this.

**Theorem 1.1.** The problem of deciding whether a given coherent configuration with maximum fiber size 4 is separable is solvable in  $\oplus L$ .

Since  $\oplus L \subseteq NC^2$  (which follows from the inclusion  $\#L \subseteq NC^2$  in [37]), Theorem 1.1 implies that the separability problem is solvable in parallel polylogarithmic time. Using the reduction (1), we obtain our result for graphs.

**Theorem 1.2.** The problem of deciding whether a given vertex-colored graph of color multiplicity 4 is amenable to 2-WL is solvable in P. This holds true also for vertex- and edge-colored directed graphs.

More precisely, the proof of Theorem 1.2 yields an algorithm deciding amenability of graphs of color multiplicity at most 4 with running time  $O(n^{2+\omega})$ , where  $\omega < 2.373$  is the exponent of fast matrix multiplication [18]. Using randomization, the running time can be improved to  $O(n^4 \log^2 n)$ .

Our results have the following consequences.

Highlighting the inherent structure of the Cai-Fürer-Immerman graphs. The essence of our proof of Theorem 1.2 is an explicit description of the class of

graphs with color multiplicity 4 that are *not* amenable to 2-WL. The Cai-Fürer-Immerman graphs of color multiplicity 4 distinctly appear here as a natural subclass, which demonstrates that the Cai-Fürer-Immerman construction is not ad hoc. In a sense, the famous CFI gadget [9, Fig. 3] (or [24, Fig. 13.24]) appears in our analysis inevitably "by itself". More precisely, this concerns a simplified version of the CFI gadget, where each vertex in a cubic pattern graph is replaced with a quadruple of new vertices and two quadruples are connected by edges directly, and not via

two extra pairs of auxiliary vertices as in the original version; cf. Figure 17. The simplified gadget appears in an algebraic analog of the CFI result by Evdokimov and Ponomarenko [14]; see also Fürer's survey paper [17]. This gadget comes out also in the *shrunken* multipede graphs [32] (we discuss the multipede graphs below). A transformation of the original CFI gadget into the simplified one is easy to retrace using the framework of coherent configuration; see Section 5 where it is shown that the auxiliary vertex pairs can be cut down in  $\mathcal{C}(G)$  without affecting the separability property.

Relevance to multipede graphs. While the CFI graphs have many automorphisms, Gurevich and Shelah [20] came up with a construction of (non-binary) multipede structures that are rigid and yet not identifiable by k-WL. Neuen and Schweitzer [32, 33] combined both approaches to construct multipede graphs and to give sufficient conditions ensuring that these graphs are not amenable to k-WL (see also a recent related paper [12]). The multipede graphs are vertex-colored and the results of [32, 33] make perfect sense if the color multiplicity is bounded by 4. We observe a close connection between such multipede graphs and the class of ir-redundant coherent configurations playing a key role in the proof of Theorem 1.1. An irredundant coherent configuration typically admits a natural representation by a multipede graph and vice versa; see Remark 9.4. Though non-amenability to k-WL for higher dimensions implies non-amenability to 2-WL, the results obtained in [12, 32, 33] and in our paper are incomparable as we provide both sufficient and necessary conditions for 2-WL-non-amenability.

More graphs hard for 2-WL. Our analysis reveals new types of non-amenable graphs. A particularly elegant construction is based on the well-studied  $(n_3)$ -configurations of lines and points [19, 34]. For example, the 7-point Fano plane and the 9-point Pappus configuration give rise to non-amenable graphs of color multiplicity 4 with, respectively, 28 and 36 vertices.

Classification of small graphs. Our amenability criteria are easy to apply in many cases. In particular, they imply that all graphs of color multiplicity 4 with no more than 15 vertices are amenable. Among graphs of color multiplicity 4 with 16 vertices there are 436 non-amenable graphs. They are split into 218 pairs of 2-WL-indistinguishable non-isomorphic graphs, where a typical instance is the pair consisting of vertex-colored Shrikhande and  $4 \times 4$  rook's graphs, which are known as the smallest pair of strongly regular graphs with the same parameters.

**Small coherent configurations.** The corresponding fact about coherent configurations is that all of them with 15 or fewer vertices and fiber size 4 are separable. This result can be obtained from our cut-down lemmas in Sections 4–6 and the known fact that all quasiregular coherent configurations with at most 3 fibers are separable [22], but we provide a self-contained proof; see Theorem 11.1. Moreover,

on 16 vertices there is a unique, up to isomorphism, non-separable coherent configuration with fiber size 4. Note that all coherent configuration with at most 15 points have been enumerated [28], but their separability analysis seems to be still missing.<sup>1</sup>

**Definability of a graph in 3-variable logic.** A graph G is definable in a logic  $\mathcal{L}$  if  $\mathcal{L}$  contains a sentence  $\Phi$  that is true on G and false on any graph H non-isomorphic to G. It is well known [9] that G is definable in (k+1)-variable first-order logic with counting quantifiers if and only if G is amenable to k-WL. The aforementioned result by Immerman and Lander [25] actually says that every graph of color multiplicity at most 3 is definable in 3-variable logic, even without counting quantifiers. Our Theorem 1.2 can be recast as follows: It can be decided in polynomial time whether a given graph of color multiplicity 4 is definable in the counting 3-variable logic.

## Structure of the paper

Our formal framework is presented in Section 2, where we give basic facts about coherent configurations and use them to prove equivalence (1).

Formally, a coherent configuration  $\mathcal{C}$  on a point set V is a partition of the Cartesian square  $V^2$ . Elements of the partition are called basis relations of  $\mathcal{C}$ . The reflexive basis relations determine a partition of V into fibers  $X_1, \ldots, X_s$ . A cell  $\mathcal{C}[X_i]$  of  $\mathcal{C}$  (or a homogeneous component of  $\mathcal{C}$ ) is formed by the basis relations that are defined on  $X_i$ . An interspace  $\mathcal{C}[X_i, X_j]$  is formed by the basis relations between  $X_i$  and  $X_j$ . A coherent configuration has the property that every basis relation belongs either to a cell or to an interspace.

In Section 3 we explore the local structure of a coherent configuration  $\mathcal{C}$  under the condition that  $|X_i| \leq 4$  for every fiber of  $\mathcal{C}$ . We call an interspace  $\mathcal{C}[X_i, X_j]$  uniform if it contains a single basis relation  $X_i \times X_j$ . We observe that a non-uniform interspace  $\mathcal{C}[X_i, X_j]$  between 4-point fibers  $X_i$  and  $X_j$  contains either a matching relation between  $X_i$  and  $X_j$  or a relation whose underlying undirected graph is an 8-cycle or the union of two 4-cycles. In the last case we say that  $\mathcal{C}[X_i, X_j]$  is an interspace of  $type\ 2K_{2,2}$ . It is known [10] (see also Subsection 3.2) that it suffices to solve the separability problem for coherent configurations that are indecomposable in a direct sum of smaller configurations. As a consequence, we can assume in our analysis that every fiber  $X_i$  consists of either 4 or 2 points; see Sections 3.1–3.2 for details.

In Sections 4–6 we prove three cut-down lemmas:

- If an interspace  $C[X_i, X_j]$  contains a matching relation, then removal of the fiber  $X_i$  from C does not affect the separability property.
- Furthermore, all fibers of size 2 can be removed without affecting the separability property.

<sup>&</sup>lt;sup>1</sup>Coherent configurations on 16 vertices were studied in [27].

• Finally, all pairs of fibers  $X_i, X_j$  such that  $\mathcal{C}[X_i, X_j]$  contains an 8-cycle can be removed without affecting the separability property.

The first cut-down lemma, allowing elimination of matching basis relations, is proved in the general case, with no assumptions on the coherent configuration  $\mathcal{C}$ . One direction, namely the non-separability of the reduced version of a non-separable configuration  $\mathcal{C}$ , was known earlier due to Evdokimov and Ponomarenko [15].

The cut-down lemmas reduce our task to consideration of indecomposable coherent configurations  $\mathcal{C}$  with all fibers of size 4 and all non-uniform interspaces of type  $2K_{2,2}$ . We call such coherent configurations irredundant. This class is close to the reduced Klein configurations studied in [10, Section 4.1.2]. The fiber graph  $F_{\mathcal{C}}$  has the fibers of  $\mathcal{C}$  as vertices, and two fibers  $X_i$  and  $X_j$  are adjacent in  $F_{\mathcal{C}}$  if the interspace  $\mathcal{C}[X_i, X_j]$  is non-uniform. Like the reduced Klein configurations, the structure of an irredundant configuration  $\mathcal{C}$  determines a clique partition  $D_{\mathcal{C}}$  of  $F_{\mathcal{C}}$  such that the cliques and the fibers form a line-point incidence structure known as partial linear spaces (see [13, 30]), where every point (fiber) is incident to at most 3 lines (cliques in  $D_{\mathcal{C}}$ ).

The case when all cliques in  $D_{\mathcal{C}}$  have size 2 corresponds to the Cai-Fürer-Immerman construction. Though coherent configurations of this kind are well studied (Evdokimov and Ponomarenko [14], see also [10, Section 4.1.3]), we consider them in Section 8 for expository purposes as the simplest case of irredundant configurations. Another instructive particular case, when all cliques in  $D_{\mathcal{C}}$  have size 3, is called 3-harmonious and considered in Section 9. The underlying partial linear spaces of such coherent configurations are the well-studied geometric  $(n_3)$ -configurations [19, 34].

After this case study, we consider the general irredundant configurations in Section 10. Note that the standard isomorphism concept of coherent configurations is called *combinatorial isomorphism*, while the equivalence with respect to the regularity parameters is captured by the concept of algebraic isomorphism. Deciding separability of an irredundant configuration  $\mathcal{C}$ , we actually have to check whether every algebraic isomorphism from  $\mathcal{C}$  to another coherent configuration  $\mathcal{C}'$  is induced by a combinatorial isomorphism. The first observation (made in Section 7), which makes our analysis easier, is that we can suppose that  $\mathcal{C}' = \mathcal{C}$ , that is, we can focus on algebraic automorphisms of  $\mathcal{C}$ . Moreover, it is enough to check only those automorphisms which fix each cell of  $\mathcal{C}$ . All such algebraic automorphisms form a group, which we denote by  $\mathbb{A}(\mathcal{C})$ . Given  $f \in \mathbb{A}(\mathcal{C})$ , we can efficiently decide whether f is induced by a combinatorial automorphism by considering suitable colored versions of  $\mathcal{C}$  and its image  $\mathcal{C}^f$  and applying the algorithm of [1] for testing isomorphism of vertex-colored graphs of color multiplicity 4. The main difficulty is that the group  $\mathbb{A}(\mathcal{C})$  can be of exponentially large order. Luckily, it is enough to consider any set of generators of  $\mathbb{A}(\mathcal{C})$  of polynomial size. We give an explicit description of an appropriate generating set based on the system of cliques  $D_{\mathcal{C}}$ .

We summarize our decision procedure in Section 11. Theorem 1.1 is proved by showing that the separability problem for irredundant configurations reduces in logarithmic space to the isomorphism problem for graphs of color multiplicity 4. Theorem 1.2 is proved in Section 12 based on Equivalence (1) and the result of [1] that isomorphism testing for graphs of color multiplicity 4 is not harder than computing the rank of a matrix over the 2-element field. Finally, we apply our amenability criteria to graphs of color multiplicity 4 with at most 16 vertices.

We conclude with a brief discussion of further questions in Section 13.

# 2 Basic definitions and facts

We begin with a formal definition of an undirected vertex-colored graph and then introduce a more general notion of a colored graph, whose edges are directed and colored (Subsection 2.1). The subsequent notion of a rainbow (Subsection 2.2) is identical at first sight but uses a different isomorphism concept. Informally speaking, rainbows are colored graphs considered up to renaming the colors. Coherent configurations are rainbows with certain regularity properties. The Weisfeiler-Leman algorithm (Subsection 2.3) converts an input graph into a coherent configuration and, moreover, furnishes this configuration with a canonical coloring. We introduce the amenability and separability concepts and reduce the former to the latter in Subsection 2.4.

# 2.1 Colored graphs

By a vertex-colored graph G we mean an undirected graph without multiple edges and loops that is endowed with a coloring of the vertex set  $c_G: V(G) \to C$ , where C is a set whose elements are called *colors*. Vertex-colored graphs G and H are isomorphic if there is a graph isomorphism  $\phi: V(G) \to V(H)$  that preserves colors, i.e.,

$$c_H(\phi(v)) = c_G(v)$$
 for all  $v \in V(G)$ .

In a more general setting, we consider directed graphs with colored edges (arrows). The loops are allowed, but the color of a loop vv must differ from the color of any arrow uw with  $u \neq w$ . This generalizes the concept of a vertex-colored graph because the colors of loops can be seen as a vertex coloring, and a symmetric adjacency relation can be simulated by requiring that uv is an arrow if any only if vu is an arrow.

In fact, we do not need an adjacency relation (symmetric or not) at all because all non-arrows can be assigned a special color. Formally, we define a *colored (directed)* graph G as a function  $c_G: V(G)^2 \to C$  such that

$$c_G(vv) \neq c_G(uw)$$
 whenever  $u \neq w$ . (2)

Two colored graphs G and H are isomorphic if there is a bijection  $\phi:V(G)\to V(H)$  such that

$$c_H(\phi(u)\phi(v)) = c_G(uv)$$
 for all  $u, v \in V(G)$ .

In the context of the isomorphism problem, we can always assume that

$$c_G(uv) = c_G(u'v') \text{ if and only if } c_G(vu) = c_G(v'u'), \tag{3}$$

that is, if arrows have the same color, then the inverse arrows must also be equally colored. This condition can be ensured by modifying the coloring as follows. Suppose that an arrow uv is colored red in G, and the inverse arrow vu is colored blue. Then uv is recolored a new color redblue, and vu is recolored a new color bluered. The new colored graph  $\hat{G}$  satisfies the condition (3). Note that  $\hat{G} \cong \hat{H}$  exactly when  $G \cong H$ . This motivates imposing the condition (3) on any colored graph.

For each color  $c \in C$ , the set  $\{uv : c_G(uv) = c\}$  is called a *color class* of G. A color class consisting of loops is referred to as *vertex color class*. We define the *color multiplicity* of G as the maximum cardinality of a vertex color class of G.

## 2.2 Coherent configurations

Let V be a set, whose elements are called *points*. Let  $C = \{R_1, \ldots, R_s\}$  be a partition of the Cartesian square  $V^2$ , that is,  $\bigcup_{i=1}^s R_i = V^2$  and any two  $R_i$  and  $R_j$  are disjoint. An element  $R_i$  of C will be referred to as a basis relation. C is called a rainbow if it has the following two properties:

- (A) If a basis relation  $R \in \mathcal{C}$  contains a loop vv, then all pairs in R are loops;
- (B) For every  $R \in \mathcal{C}$ , the transpose relation  $R^* = \{uv : vu \in R\}$  is also in  $\mathcal{C}$ .

Though formally a rainbow is a pair  $(V, \mathcal{C})$ , we simplify the notation by using the same character  $\mathcal{C}$  for the rainbow and its set of basis relations. This will cause no ambiguity as the point set  $V = V(\mathcal{C})$  is uniquely determined as the set of all elements occurring in the relations from  $\mathcal{C}$ .

A set of points  $X \subseteq V$  is called a *fiber* of  $\mathcal{C}$  if the set of loops  $\{xx : x \in X\}$  is a basis relation of  $\mathcal{C}$ .

Two rainbows (or, more generally, two partitions)  $\mathcal{C}$  and  $\mathcal{D}$  are isomorphic if there is a bijection  $\phi: V(\mathcal{C}) \to V(\mathcal{D})$ , an isomorphism from  $\mathcal{C}$  to  $\mathcal{D}$ , such that  $\phi(R) \in \mathcal{D}$  for every  $R \in \mathcal{C}$ . Here  $\phi(R) = \{\phi(u)\phi(v) : uv \in R\}$ . We can sometimes write the same as  $R^{\phi} = \{u^{\phi}v^{\phi} : uv \in R\}$ .

Note that Conditions (A) and (B) are analogs of Conditions (2) and (3). By this reason, a colored graph will also be called a *colored rainbow*. Let G be a colored graph and  $\mathcal{C}$  be a rainbow. If  $V(G) = V(\mathcal{C})$  and the color classes of G are exactly the basis relations of  $\mathcal{C}$ , then we say that G is a *colored version* of  $\mathcal{C}$ . Thus, rainbows  $\mathcal{C}$  and  $\mathcal{D}$  are isomorphic if and only if they have colored versions that are isomorphic (as colored graphs).

A rainbow C is called a coherent configuration if,

(C) for every triple  $R, S, T \in \mathcal{C}$ , the number  $p(uv) = |\{w : uw \in R, wv \in S\}|$  is the same for all  $uv \in T$ .

For a coherent configuration C, the number p(uv) in (C) does not depend on the choice of uv in T and is denoted by  $p_{RS}^T$ . The entries of this 3-dimensional matrix are called *intersection numbers* of C.

Coherent configurations  $\mathcal{C}$  and  $\mathcal{D}$  are combinatorially isomorphic if they are isomorphic as rainbows. We write  $\mathcal{C} \cong_{comb} \mathcal{D}$  for this relationship. Correspondingly, any isomorphism from  $\mathcal{C}$  to  $\mathcal{D}$  is called combinatorial. Coherent configurations  $\mathcal{C}$  and  $\mathcal{D}$  are algebraically isomorphic if their 3-dimensional matrices of intersection numbers,  $p_{RS}^T$  and  $p_{R'S'}^{T'}$ , are isomorphic, that is, there is a bijection  $f: \mathcal{C} \to \mathcal{D}$  such that

$$p_{RS}^T = p_{f(R)f(S)}^{f(T)}.$$

In this case we write  $\mathcal{C} \cong_{alg} \mathcal{D}$ . Such a bijection f is called an algebraic isomorphism from  $\mathcal{C}$  to  $\mathcal{D}$ . Note that combinatorially isomorphic coherent configurations are also algebraically isomorphic. Indeed, any combinatorial isomorphism  $\phi$  from  $\mathcal{C}$  to  $\mathcal{D}$  gives rise to the algebraic isomorphism f defined by  $f(R) = R^{\phi}$ .

Let  $A_R$  denote the adjacency matrix of a relation  $R \subseteq V^2$ , i.e.,  $A_R[u, v]$  is equal to 1 if  $uv \in R$  and to 0 otherwise. Define  $\mathcal{A}_{\mathcal{C}}$  to be the linear span of the set of 0-1-matrices  $\{A_R : R \in \mathcal{C}\}$  over  $\mathbb{C}$ . Condition (C) implies that  $\mathcal{A}_{\mathcal{C}}$  is closed under matrix multiplication and, hence, forms a matrix algebra over  $\mathbb{C}$ . This algebra is called the adjacency algebra of the coherent configuration  $\mathcal{C}$ . It turns out [10, Proposition 2.3.17] that coherent configurations  $\mathcal{C}$  and  $\mathcal{D}$  are algebraically isomorphic if and only if  $\mathcal{A}_{\mathcal{C}}$  and  $\mathcal{A}_{\mathcal{D}}$  are isomorphic algebras with distinguished bases. Another important characterization of algebraic isomorphism will be given in Subsection 2.3.

Given a family of sets  $\mathcal{P}$ , we use  $\mathcal{P}^{\cup}$  to denote the closure of  $\mathcal{P}$  under unions. Given two partitions  $\mathcal{P}$  and  $\mathcal{Q}$  of the same set, we write  $\mathcal{P} \leq \mathcal{Q}$  if every set in  $\mathcal{Q}$  belongs to  $\mathcal{P}^{\cup}$  or, equivalently, every set in  $\mathcal{P}$  is a subset of some set in  $\mathcal{Q}$ . In this case we say that  $\mathcal{P}$  is finer than  $\mathcal{Q}$  and  $\mathcal{Q}$  is coarser than  $\mathcal{P}$ .

**Proposition 2.1** (see [10, Section 2.6.1]). Let  $\mathcal{P}$  be a partition of the Cartesian square  $V^2$ . Then there is a unique coherent configuration  $\mathcal{C} = \mathcal{C}(\mathcal{P})$  such that

- $\mathcal{C} \preceq \mathcal{P}$ , and
- if C' is a coherent configuration such that  $C' \leq P$ , then  $C' \leq C$ .

The coherent configuration  $\mathcal{C}(\mathcal{P})$  is called the *coherent closure* of  $\mathcal{P}$ . In other words, the coherent closure of  $\mathcal{P}$  is the coarsest of those coherent configurations refining  $\mathcal{P}$ . Given a colored (directed) graph G (in particular, a vertex-colored undirected graph), let  $\mathcal{R}_G$  denote its uncolored version, that is, the rainbow whose basis relations are exactly the color classes of G. The coherent configuration  $\mathcal{C}(\mathcal{R}_G)$  is called the *coherent closure of the graph* G and denoted by  $\mathcal{C}(G)$ .

The following notational convention will be intensively used till the end of this section. Suppose that  $\mathcal{P}$  and  $\mathcal{Q}$  are partitions. Any map  $f: \mathcal{P} \to \mathcal{Q}$  extends to a map from  $\mathcal{P}^{\cup}$  to  $\mathcal{Q}^{\cup}$  in a natural way. Specifically, if  $X = X_1 \cup \ldots \cup X_s$  where  $X_i \in \mathcal{P}$ , then  $X^f = X_1^f \cup \ldots \cup X_s^f$ . Usage of the superscript f can be extended as usually: If  $\mathcal{X} = \{X_1, \ldots, X_q\}$  where  $X_i \in \mathcal{P}^{\cup}$ , then  $\mathcal{X}^f = \{X_1^f, \ldots, X_q^f\}$ . Note that, if  $f: \mathcal{P} \to \mathcal{Q}$  is a bijection and  $\mathcal{P} \preccurlyeq \mathcal{R}$ , then  $\mathcal{Q} \preccurlyeq \mathcal{R}^f$ .

**Lemma 2.2** (see [10, Corollary 2.3.21]). If f is an algebraic isomorphism from a coherent configuration  $\mathcal{P}$  to a coherent configuration  $\mathcal{Q}$ , and  $\mathcal{R}$  is a coherent configuration such that  $\mathcal{P} \preceq \mathcal{R}$ , then  $\mathcal{R}^f$  is also a coherent configuration.

## 2.3 The Weisfeiler-Leman algorithm

The following algorithm, that was described by Weisfeiler and Leman in [36], is now known as the 2-dimensional Weisfeiler-Leman algorithm (2-WL for short). Given a colored graph G as input, the algorithm iteratively computes colorings  $c_G^i$  of the Cartesian square  $V^2$  for V = V(G). Initially,  $c_G^0 = c_G$  and then,

$$c_G^{i+1}(uv) = c_G^i(uv) \mid \{ \{ c_G^i(uw) \mid c_G^i(wv) \} \}_{w \in V},$$
(4)

where  $\{\!\{\}\!\}$  denotes the multiset and | denotes the string concatenation (an appropriate encoding is assumed). Denote the partition of  $V^2$  into the color classes of  $c_G^i$  by  $\mathcal{R}_G^i$ . Note that  $\mathcal{R}_G^{i+1} \preccurlyeq \mathcal{R}_G^i$ . Let  $t=t_G$  be the minimum number such that  $\mathcal{R}_G^t = \mathcal{R}_G^{t-1}$ . The algorithm terminates after the t-th color refinement round. As easily seen,  $\mathcal{R}_G^t$  is a coherent configuration.<sup>2</sup>

**Proposition 2.3** (see [10, Section 2.6.1]).  $\mathcal{R}_G^t = \mathcal{C}(G)$ .

An easy induction on i shows that, if  $\phi$  is an isomorphism from G to H, then

$$c_G^i(uv) = c_H^i(u^\phi v^\phi). (5)$$

Thus, the coloring produced by 2-WL is canonical and can be used for isomorphism testing. We say that colored graphs G and H are 2-WL-equivalent and write  $G \equiv_{2\text{-WL}} H$  if

$$\{ c_G^t(uv) : uv \in V(G)^2 \} = \{ c_H^t(uv) : uv \in V(H)^2 \}$$
(6)

for  $t = t_G$  (equivalently, for  $t = t_H$ , or for all t).

Suppose that  $G \equiv_{2\text{-WL}} H$ . Equality (6) implies that there is a one-to-one map f:  $\mathcal{C}(G) \to \mathcal{C}(H)$  preserving the 2-WL colors. Note that f is an algebraic isomorphism from  $\mathcal{C}(G)$  to  $\mathcal{C}(H)$ . We, therefore, have the following diagram:

$$\begin{array}{ccc} G \cong H & \Longrightarrow & G \equiv_{\text{2-WL}} H \\ & & & & \downarrow \\ \mathcal{C}(G) \cong_{comb} \mathcal{C}(H) & \Longrightarrow & \mathcal{C}(G) \cong_{alg} \mathcal{C}(H) \end{array}$$

In the other direction, let f be an algebraic isomorphism from  $\mathcal{C}$  to  $\mathcal{D}$ . If  $\tilde{\mathcal{C}}$  is a colored version of  $\mathcal{C}$ , and  $\tilde{\mathcal{D}}$  is the colored version of  $\mathcal{D}$  where each color class f(C) inherits the color of C, then  $\tilde{\mathcal{C}} \equiv_{2\text{-WL}} \tilde{\mathcal{D}}$ . Thus, the Weisfeiler-Leman algorithm provides yet another interpretation for algebraic isomorphism of coherent configurations:  $\mathcal{C} \cong_{alg} \mathcal{C}$ 

<sup>&</sup>lt;sup>2</sup>Moreover, a partition  $\mathcal{P}$  is a coherent configuration if and only if 2-WL does not make any color refinement when applied to a colored version of  $\mathcal{P}$ .

 $\mathcal{D}$  if and only if  $\mathcal{C}$  and  $\mathcal{D}$  have colored versions  $\tilde{\mathcal{C}}$  and  $\tilde{\mathcal{D}}$  respectively such that  $\tilde{\mathcal{C}} \equiv_{2\text{-WL}} \tilde{\mathcal{D}}$ .

The fact that the 2-WL-equivalence of graphs G and H determines an algebraic isomorphism of their coherent closures  $\mathcal{C}(G)$  and  $\mathcal{C}(H)$  has the converse, which we state now.

**Lemma 2.4.** Let  $\mathcal{P}$  and  $\mathcal{Q}$  be rainbows and  $f: \mathcal{C}(\mathcal{P}) \to \mathcal{C}(\mathcal{Q})$  be an algebraic isomorphism such that  $\mathcal{Q} = \mathcal{P}^f$ . Let G be a colored version of  $\mathcal{P}$ . Let H be the colored version of  $\mathcal{Q}$  that inherits the colors from G via f, that is, every color class C of G has the same color as the color class  $C^f$  of H.

- **1.** If 2-WL is run on G (resp. H), then it outputs a colored version of C(P) (resp. C(Q)).
- **2.** The map f preserves the 2-WL coloring, that is,

$$c_G^i(Z) = c_H^i(Z^f) \tag{7}$$

for all  $i \geq 0$  and  $Z \in \mathcal{C}(\mathcal{P})$ , where  $c_G^i(Z) := c_G^i(uv)$  for an arrow uv in Z and  $c_H^i(Z^f)$  is defined similarly. In particular,  $G \equiv_{2\text{-WL}} H$ .

**3.** If, moreover,  $G \cong H$ , then f is induced by a combinatorial isomorphism from  $\mathcal{C}(\mathcal{P})$  to  $\mathcal{C}(\mathcal{Q})$ .

*Proof.* 1. This part follows directly from Proposition 2.3.

2. We use the induction on i. For i=0, Equality (7) follows from the fact that the coloring of H is defined according to the map f. Assume that Equality (7) is true for some value of i for all  $Z \in \mathcal{C}(\mathcal{P})$  and prove that then  $c_G^{i+1}(Z) = c_H^{i+1}(Z^f)$  for all  $Z \in \mathcal{C}(\mathcal{P})$ . Choose arbitrarily an arrow uv in Z and an arrow u'v' in  $Z^f$ . It suffices to prove that

$$\{ \{ c_G^i(uw) \mid c_G^i(wv) \} \}_{w \in V(G)} = \{ \{ c_H^i(u'w') \mid c_H^i(w'v') \} \}_{w' \in V(H)}.$$
 (8)

Each pair  $X,Y \in \mathcal{C}(\mathcal{P})$  contributes  $p_{XY}^Z$  elements  $c_G^i(X) \mid c_G^i(Y)$  into the left-hand side of (8). Similarly, for each  $X,Y \in \mathcal{C}(\mathcal{P})$ , the right-hand side of (8) contains  $p_{f(X)f(Y)}^{f(Z)}$  elements  $c_H^i(X^f) \mid c_H^i(Y^f)$ . Since f is an algebraic isomorphism,

$$p_{f(X)f(Y)}^{f(Z)} = p_{XY}^Z.$$

By the induction assumption,

$$c_H^i(X^f) \mid c_H^i(Y^f) = c_G^i(X) \mid c_G^i(Y).$$

Equality (8) follows.

3. Let  $\phi$  be an isomorphism from G to H. By (5),  $\phi$  preserves the 2-WL coloring and, therefore, every X in  $\mathcal{C}(\mathcal{P})$  has the same 2-WL color as  $X^{\phi}$  in  $\mathcal{C}(\mathcal{Q})$ . By Part 2, also  $X^f$  has this color. This implies that  $X^f = X^{\phi}$ . It remains to note that  $\phi$  is a combinatorial isomorphism from  $\mathcal{C}(\mathcal{P})$  to  $\mathcal{C}(\mathcal{Q})$  (which readily follows from the fact that  $\phi$  preserves the 2-WL coloring).

# 2.4 Amenability to 2-WL and separability of the coherent closure

We call a colored graph G amenable (to 2-WL) if 2-WL distinguishes G from any non-isomorphic graph H, that is,  $G \equiv_{2\text{-WL}} H$  implies  $G \cong H$ .

A coherent configuration  $\mathcal{C}$  is *separable* if every algebraic isomorphism from  $\mathcal{C}$  to any coherent configuration  $\mathcal{D}$  is induced by a combinatorial isomorphism from  $\mathcal{C}$  to  $\mathcal{D}$ .

**Theorem 2.5.** A colored graph G is amenable if and only if its coherent closure C(G) is separable.

Proof. ( $\iff$ ) Suppose that  $G \equiv_{2\text{-WL}} H$ . Consider the map  $f : \mathcal{C}(G) \to \mathcal{C}(H)$  taking each  $X \in \mathcal{C}(G)$  to the basis relation in  $\mathcal{C}(H)$  with the same 2-WL color. This map is an algebraic isomorphism from  $\mathcal{C}(G)$  to  $\mathcal{C}(H)$ . Since  $\mathcal{C}(G)$  is separable, f is induced by a combinatorial isomorphism  $\phi$  from  $\mathcal{C}(G)$  to  $\mathcal{C}(H)$ . Since  $\phi$  preserves the 2-WL coloring  $c_G^t$ , it preserves also the initial coloring  $c_G^0$ , which means that  $\phi$  is an isomorphism from G to G.

 $(\Longrightarrow)$  Given an algebraic isomorphism  $f:\mathcal{C}(G)\to\mathcal{D}$ , we have to show that f is induced by a combinatorial isomorphism from  $\mathcal{C}(G)$  to  $\mathcal{D}$ . Let  $\mathcal{R}$  denote the rainbow which is the uncolored version of G.

Claim A.  $\mathcal{D} = \mathcal{C}(\mathcal{R}^f)$ .

Proof of Claim A. Since  $\mathcal{C}(\mathcal{R}) \leq \mathcal{R}$ , we have  $\mathcal{D} \leq \mathcal{R}^f$ . By Proposition 2.1, this implies that  $\mathcal{D} \leq \mathcal{C}(\mathcal{R}^f)$ . Applying the inverse map  $f^{-1}: \mathcal{D}^{\cup} \to \mathcal{C}(G)^{\cup}$ , we have

$$C(\mathcal{R}) \preceq (C(\mathcal{R}^f))^{f^{-1}}.$$
 (9)

Since  $f^{-1}$  is an algebraic isomorphism from  $\mathcal{D}$  to  $\mathcal{C}(\mathcal{R})$ , Lemma 2.2 implies that  $(\mathcal{C}(\mathcal{R}^f))^{f^{-1}}$  is a coherent configuration. Since  $f^{-1}$  takes  $\mathcal{R}^f$  back to  $\mathcal{R}$ , we have

$$(\mathcal{C}(\mathcal{R}^f))^{f^{-1}} \preccurlyeq \mathcal{R}$$

and, by Proposition 2.1,

$$(\mathcal{C}(\mathcal{R}^f))^{f^{-1}} \preccurlyeq \mathcal{C}(\mathcal{R}).$$

Along with (9), this shows that  $(\mathcal{C}(\mathcal{R}^f))^{f^{-1}} = \mathcal{C}(\mathcal{R})$  or, equivalently,  $\mathcal{C}(\mathcal{R}^f) = \mathcal{C}(\mathcal{R})^f = \mathcal{D}$ .

Let  $G^f$  denote the colored version of  $\mathcal{R}^f$  that inherits the colors of G according to the bijection  $f: \mathcal{R} \to \mathcal{R}^f$ . Using Claim A and Part 2 of Lemma 2.4, we conclude that  $G \equiv_{2\text{-WL}} G^f$ . Since G is amenable,  $G \cong G^f$ . By Part 3 of Lemma 2.4, the algebraic isomorphism f is induced by a combinatorial isomorphism from  $\mathcal{C}(G)$  to  $\mathcal{D}$ .

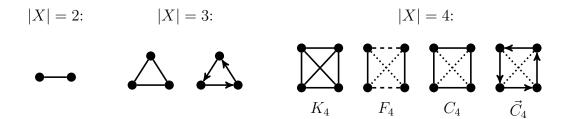


Figure 1: Cells  $\mathcal{C}[X]$  on 2, 3, and 4 points.

# 3 Preliminaries on the structure of coherent configurations

## 3.1 Fibers and interspaces

Let  $\mathcal{C}$  be a coherent configuration on the point set  $V = V(\mathcal{C})$ . Recall that a set of points  $X \subseteq V$  is a fiber of  $\mathcal{C}$  if it underlies a reflexive basis relation of  $\mathcal{C}$ . Denote the set of all fibers of  $\mathcal{C}$  by  $F(\mathcal{C})$ . By Property (A) in Section 2.2,  $F(\mathcal{C})$  is a partition of V. Property (C) implies that for every basis relation R of  $\mathcal{C}$  there are, not necessarily distinct, fibers X and Y such that  $R \subseteq X \times Y$ . Thus, if  $X, Y \in F(\mathcal{C})$ , then the Cartesian product  $X \times Y$  is split into basis relations of  $\mathcal{C}$ . We denote this partition by  $\mathcal{C}[X,Y]$ . If X = Y, we simplify our notation to  $\mathcal{C}[X] = \mathcal{C}[X,X]$ . Note that  $\mathcal{C}[X]$  is a coherent configuration on X, with X being its single fiber. We will call  $\mathcal{C}[X]$  a cell of  $\mathcal{C}$ . In general, coherent configurations with a single fiber are called association schemes.

All possible association schemes on 2, 3, and 4 points are depicted in Figure 1. Undirected edges are used to show basis relations that are equal to their transposes. Directed edges are used to show basis relations that are not equal to their transposes, and those are then not shown as they are reconstructable by reversing the arrows. Loops are not shown at all. Though we use different patterns for different basis relations, remember that C[X] is just an (uncolored) partition of X. We give the 4-point cells names  $K_4$ ,  $C_4$ ,  $\vec{C}_4$ , and  $F_4$  according to the names of the graphs appearing as underlying shapes in the cell representations. Here,  $\vec{C}_4$  stands for the directed 4-cycle, and  $F_4$  stands for the factorization of the complete graph  $K_4$  into three matchings  $2K_2$ . We use notation  $C[X] \simeq C_4$  etc. to indicate which type the cell C[X] has.

If  $X \neq Y$ , we call the partition  $\mathcal{C}[X,Y]$  an *interspace* of  $\mathcal{C}$ . Note that  $R \in \mathcal{C}[X,Y]$  if and only if  $R^* \in \mathcal{C}[Y,X]$ . In particular,  $R \in \mathcal{C}[X,Y]$  for  $X \neq Y$  implies that  $R^* \neq R$ . If  $|\mathcal{C}[X,Y]| = 1$ , that is,  $X \times Y$  is a basis relation of  $\mathcal{C}$ , then the interspace  $\mathcal{C}[X,Y]$  will be called *uniform*. Otherwise,  $\mathcal{C}[X,Y]$  will be referred to as *non-uniform*. The interspace  $\mathcal{C}[X,Y]$  is uniform if and only if so is  $\mathcal{C}[Y,X]$ .

If  $R \in \mathcal{C}[X,Y]$ , then the number of arrows in R from a point  $x \in X$  is the same for each x in X. We call this number the valency of R and denote it by d(R).

**Lemma 3.1.** Let  $X, Y \in F(\mathcal{C})$ . If |X| and |Y| are coprime, then  $\mathcal{C}[X, Y]$  is uniform.

*Proof.* Let R be a basis relation such that  $R \subseteq \mathcal{C}[X,Y]$ . Recall that the valency d(R) is equal to the number of arrows in R from each point  $x \in X$ . Note also that the valency  $d(R^*)$  of the transpose relation  $R^*$  is equal to the number of arrows in R to a point  $y \in Y$ ; it does not depend on the choice of y. It follows that

$$d(R)|X| = |R| = d(R^*)|Y|.$$

Since |X| and |Y| are coprime, d(R) is divisible by |Y|. Taking into account that  $d(R) \leq |Y|$ , we obtain the equality d(R) = |Y|. As a consequence,  $R = X \times Y$ .  $\square$ 

Thus, all interspaces C[X,Y] with |X|=1 are uniform, and so are also interspaces with |X|=2 and |Y|=3. Figure 2 shows all non-uniform interspaces C[X,Y] with  $|X|\leq 3$  and  $|Y|\leq 3$ . Here we adhere to the following convention: A pair xy with  $x\in X$  in  $y\in Y$  is shown as an undirected edge, as it is automatically ordered once the ordered pair of fibers X,Y is given. To facilitate visualization, one basis relation in each picture is not shown. It is reconstructable by taking the bipartite complement of the shown part.

If we allow also fibers on 4 points, then the list of all non-uniform interspaces (up to isomorphism of partitions) is completed in Figure 3. Again, one basis relation is not shown in each case as it is reconstructable by taking the bipartite complement. If |X| < |Y| = 4, then Lemma 3.1 implies that a non-uniform interspace  $\mathcal{C}[X,Y]$  is possible only for |X|=2. Such an interspace is unique. Suppose that |X|=|Y|=4. As agreed, we represent a basis relation as an undirected bipartite graph with vertex classes X and Y (tacitly assuming the arrows in the direction from X to Y). Note that this graph must be regular. There is a unique basis relation of degree 1 (a 4-matching), a unique basis relation of degree 3 (the bipartite complement of a 4matching), and there are two self-complementary basis relations of degree 2 (two disjoint 4-cycles and a 8-cycle). This yields three non-uniform interspaces  $\mathcal{C}[X,Y]$ with 2 basis relations, for which we will use names  $4K_{1,1}$ ,  $2K_{2,2}$ , and  $C_8$ , using the notation  $\mathcal{C}[X,Y] \simeq 2K_{2,2}$  etc. An interspace  $\mathcal{C}[X,Y]$  with  $|\mathcal{C}[X,Y]| = 3$  consists of two basis relations of degree 1 and one basis relation of degree 2. The latter can be either an 8-cycle or the disjoint union of two 4-cycles. In each case, the two basis relations of degree 1 are obtainable in a unique, up to combinatorial isomorphism,

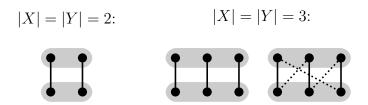


Figure 2: Non-uniform interspaces between fibers with at most 3 points.

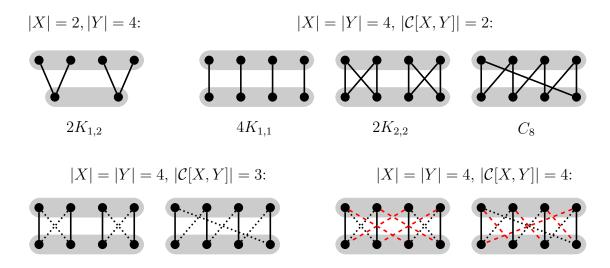


Figure 3: Non-uniform interspaces between fibers with at most 4 points.

way by splitting the complement into two 4-matchings. This yields two interspaces shown in Figure 3. An interspace C[X,Y] with |C[X,Y]| = 4 is a factorization of  $X \times Y$  into four 4-matchings. One factor is unique up to isomorphism. Two factors can form together either an 8-cycle or the disjoint union of two 4-cycles, as shown in the picture for the preceding case of |C[X,Y]| = 3. The bipartite complement of an 8-cycle is also an 8-cycle, which is uniquely factorizable into two further 4-matchings, and, therefore, C[X,Y] is uniquely determined in this case. The bipartite complement of two 4-cycles also consists of two 4-cycles. It is factorizable in two ways, but one of them leads to two 4-cycles whose union is an 8-cycle, which is the case we already have. Thus, there are two interspaces with |C[X,Y]| = 4, one with two factors forming an 8-cycle and one with every two factors forming two 4-cycles.

#### 3.2 Direct sums

Extending our notation, for any  $U \in F(\mathcal{C})^{\cup}$  we let  $\mathcal{C}[U]$  denote the set of all basis relations of  $\mathcal{C}$  contained in  $U^2$ . Note that  $\mathcal{C}[U]$  is a coherent configuration on the point set U. Let  $W = V \setminus U$ . We say that  $\mathcal{C}$  is the *direct sum* of coherent configurations  $\mathcal{C}[U]$  and  $\mathcal{C}[W]$  and write  $\mathcal{C} = \mathcal{C}[U] \boxplus \mathcal{C}[W]$  if the interspace  $\mathcal{C}[X,Y]$  is uniform for every two fibers  $X, Y \in F(\mathcal{C})$  such that  $X \subseteq U$  and  $Y \subseteq W$ .

**Lemma 3.2** (see [10, Corollary 3.2.8]). Suppose that  $C = C_1 \boxplus C_2$ . The coherent configuration C is separable if and only if both  $C_1$  and  $C_2$  are separable.

Lemma 3.2 reduces the general separability problem to its restriction for *inde-composable* coherent configurations, that is, those configurations which cannot be split into a direct sum. Lemma 3.1 implies that an indecomposable coherent configuration of maximum fiber size at most 4 either has maximum fiber size at most 3 or has only fibers of size 4 or 2.

## 3.3 Algebraic isomorphisms and fibers

**Lemma 3.3** (see [10, Proposition 2.3.18]). Let  $f: \mathcal{C} \to \mathcal{C}'$  be an algebraic isomorphism of coherent configurations. If R is a reflexive basis relations of  $\mathcal{C}$ , then  $R^f$  is a reflexive basis relations of  $\mathcal{C}'$ .

Given an algebraic isomorphism  $f: \mathcal{C} \to \mathcal{C}'$  and a fiber  $X \in F(\mathcal{C})$ , we will write f(X) to denote the fiber of  $\mathcal{C}'$  underlying the reflexive basis relation  $R^f \in \mathcal{C}'$  for the reflexive basis relation  $R = \{xx : x \in X\}$  in  $\mathcal{C}$ . Thus, the algebraic isomorphism f determines a bijection  $X \mapsto f(X)$  from  $F(\mathcal{C})$  to  $F(\mathcal{C}')$ .

As it follows directly from the definitions, whenever we want to check that a given rainbow is a coherent configuration or that a given map is an algebraic isomorphism of coherent configurations, this is enough to do locally for every triple of fibers. We formalize this observation as follows.

**Lemma 3.4.** Let C be a coherent configuration and C' be a rainbow. Let  $f: C \to C'$  be a bijection that induces a one-to-one correspondence between the reflexive relations of C and the reflexive relations of C', that is, establishes a bijection  $f: F(C) \to F(C')$ . If  $C'[f(A) \cup f(B) \cup f(C)]$  is a coherent configuration for any fibers  $A, B, C \in F(C)$  and, moreover, the restriction of f to  $C[A \cup B \cup C]$  is an algebraic isomorphism from  $C[A \cup B \cup C]$  to  $C'[A' \cup B' \cup C']$ , then C' is also a coherent configuration and f is an algebraic isomorphism from C to C'.

Lemma 3.4 readily implies the following fact. Let  $\mathcal{C}$  be a coherent configuration on point set V. For  $X \in F(\mathcal{C})$ , we denote  $\mathcal{C} \setminus X = \mathcal{C}[V \setminus X]$ .

**Lemma 3.5.** Let  $f: \mathcal{C} \to \mathcal{C}'$  be an algebraic isomorphism of coherent configurations. If  $X \in F(\mathcal{C})$ , then the restriction of f to  $\mathcal{C} \setminus X$  is an algebraic isomorphism from  $\mathcal{C} \setminus X$  to  $\mathcal{C}' \setminus f(X)$ .

# 4 Cutting it down: Interspaces with a matching

Let M be a basis relation of a coherent configuration  $\mathcal{C}$ . Suppose that  $M \in \mathcal{C}[X,Y]$  for distinct fibers X and Y. We call M a matching if both M and its transpose have valency 1, i.e.,  $d(M) = d(M^*) = 1$ . This means that M determines a one-to-one correspondence between X and Y. In the case that  $M \in \mathcal{C}[X]$  for a fiber X, we call M a matching if  $d(M) = d(M^*) = 1$  and, additionally, M is symmetric and irreflexive. In this case, M determines a partition of X into pairs of points.

**Lemma 4.1.** Suppose that a coherent configuration C contains a matching basis relation in an interspace C[X,Y]. Then C is separable if and only if  $C \setminus X$  is separable.

We split the proof of Lemma 4.1 into two parts, Lemmas 4.6 and 4.8 below.

Before proceeding to the proof, we need some definitions. We call a rainbow  $\mathcal{P}$  fibrous if for every basis relation  $R \in \mathcal{P}$  there are, not necessarily distinct, fibers  $X, Y \in F(\mathcal{P})$  such that  $R \subseteq X \times Y$ . Note that a coherent configuration is a fibrous rainbow. For a fibrous rainbow  $\mathcal{P}$ , we can use the notation  $\mathcal{P}[X,Y] = \{R \in \mathcal{P} : R \subseteq X \times Y\}$ , that was introduced for coherent configurations.

Let  $\mathcal{P}$  be a rainbow on point set V and  $\mathcal{Q}$  be a rainbow on point set U. We call a surjective function  $\nu: V \to U$  a folding map from  $\mathcal{P}$  to  $\mathcal{Q}$  if

- $R^{\nu} \in \mathcal{Q}$  for every basis relation  $R \in \mathcal{P}$ , and
- $|R^{\nu}| = |R|$  for every reflexive basis relation  $R \in \mathcal{P}$ .

Note that, by the first condition, for every fiber X of  $\mathcal{P}$ , its image  $X^{\nu}$  is a fiber of  $\mathcal{Q}$ . Taking into account the second condition, we see that the restriction of  $\nu$  to X is a bijection from X to  $X^{\nu}$ . Therefore, for every two (not necessarily distinct) fibers  $X, Y \in F(\mathcal{P})$ , the map  $\nu$  induces a bijection from  $X \times Y$  onto  $X^{\nu} \times Y^{\nu}$ . If  $\mathcal{P}$  is fibrous, this implies that  $\nu$ , extended to a map from  $V^2$  to  $U^2$ , induces a bijection from R to  $R^{\nu}$  for each  $R \in \mathcal{P}$ . Moreover,  $\nu$  determines a one-to-one correspondence  $R \mapsto R^{\nu}$  between  $\mathcal{P}[X,Y]$  and  $\mathcal{Q}[X^{\nu},Y^{\nu}]$  (hence  $\mathcal{Q}$  must be fibrous too).

We say that basis relations R, S, T of a fibrous rainbow  $\mathcal{P}$  form a collocated triple (or are collocated) if there are fibers  $X, Y, Z \in F(\mathcal{P})$ , not necessarily distinct, such that  $T \in \mathcal{P}[X, Y]$ ,  $R \in \mathcal{P}[X, Z]$ , and  $S \in \mathcal{P}[Z, Y]$ . If  $\mathcal{P}$  is a coherent configuration and R, S, T are not collocated, then obviously  $p_{RS}^T = 0$ .

**Lemma 4.2.** If Q is a coherent configuration and  $\nu$  is a folding map from a fibrous rainbow P to Q, then P is also a coherent configuration. Moreover,

$$p_{RS}^T = p_{R^{\nu}S^{\nu}}^{T^{\nu}}$$

for every collocated triple  $R, S, T \in \mathcal{P}$ .

Proof. If  $R, S, T \in \mathcal{P}$  are not collocated, then  $p_{RS}^T$  is obviously well defined and equal to 0, which means that Condition (C) in the definition of a coherent configuration is fulfilled for such triples. Suppose that R, S, T is a collocated triple in  $\mathcal{P}$  and that this is certified by the fibers  $X, Y, Z \in F(\mathcal{P})$ . Note that  $R^{\nu}, S^{\nu}, T^{\nu}$  is a collocated triple in  $\mathcal{Q}$ , which is certified by fibers  $X^{\nu}, Y^{\nu}, Z^{\nu} \in F(\mathcal{Q})$ . Let  $xy \in T$  and consider the set W of all  $z \in Z$  such that  $xz \in R$  and  $zy \in S$ . Note that  $z \in W$  if and only if  $x^{\nu}z^{\nu} \in R^{\nu}$  and  $z^{\nu}y^{\nu} \in S^{\nu}$ . Since  $x^{\nu}y^{\nu} \in T^{\nu}$  and  $\nu$  is a bijection from Z onto  $Z^{\nu}$ , we conclude that  $|W| = p_{R^{\nu}S^{\nu}}^{T^{\nu}}$ , not depending on the choice of xy in T.

Note that matching basis relations are *thin* in the sense of [10] and, therefore, Part 1 of the following lemma can also be obtained from [10, Example 2.2.2].

**Lemma 4.3.** Suppose that an interspace C[X,Y] of a coherent configuration C contains a matching basis relation M and define a function  $\nu:V(C)\to V(C)\setminus X$  by  $\nu(x)=y$  for all  $xy\in M$  and  $\nu(z)=z$  for all  $z\notin X$ . Then the following is true:

- **1.**  $\nu$  is a combinatorial isomorphism from the cell  $\mathcal{C}[X]$  to the cell  $\mathcal{C}[Y]$ .
- **2.** If  $R \in \mathcal{C}[X,Y] \cup \mathcal{C}[Y,X]$ , then  $R^{\nu} \in \mathcal{C}[Y]$ .
- **3.** If  $R \in \mathcal{C}[X,Z] \cup \mathcal{C}[Z,X]$ , where  $Z \in F(\mathcal{C})$  and  $Z \neq X,Y$ , then  $R^{\nu} \in \mathcal{C}[Y,Z] \cup \mathcal{C}[Z,Y]$ .
- **4.**  $\nu$  is a folding map from  $\mathcal{C}$  to  $\mathcal{C} \setminus X$ .

*Proof.* Note that  $\nu$  maps each fiber of  $\mathcal{C}$  bijectively onto a fiber of  $\mathcal{C} \setminus X$ . Throughout this proof, we write  $ab \approx a'b'$  in the case that the pairs ab and a'b' are in the same basis relation of  $\mathcal{C}$ .

1. We show that  $\nu$  takes the partition  $\mathcal{C}[X]$  of  $X^2$  onto the partition  $\mathcal{C}[Y]$  of  $Y^2$ . Let  $x_1x_2$  and  $x_3x_4$  be two, not necessarily disjoint, pairs of points of X. Denote  $y_i = \nu(x_i)$  for  $i \leq 4$ . Assuming that

$$x_1 x_2 \approx x_3 x_4,\tag{10}$$

we need to show that

$$y_1 y_2 \approx y_3 y_4. \tag{11}$$

Since  $x_1y_1$  is the only arrow in M from  $x_1$  and  $x_3y_3$  is the only arrow in M from  $x_3$ , Property (C) of a coherent configuration allows us to deduce from (10) that

$$y_1 x_2 \approx y_3 x_4. \tag{12}$$

Since  $x_2y_2$  is the only arrow in M from  $x_2$  and  $x_4y_4$  is the only arrow in M from  $x_4$ , the relation (12) along with Property (C) implies that  $y_2y_1 \approx y_4y_3$ , which implies (11) by Property (B) of a coherent configuration.

2. Suppose that  $R \in \mathcal{C}[X,Y]$  (the case  $R \in \mathcal{C}[Y,X]$  is symmetric). Note that  $\nu$  induces a bijection from  $X \times Y$  onto  $Y^2$ . Therefore, it suffices to prove that for arbitrary  $x_1, x_2 \in X$  and  $y_1, y_2 \in Y$ :

$$x_1y_1 \approx x_2y_2 \iff x_1^{\nu}y_1 \approx x_2^{\nu}y_2.$$

This readily follows from the fact  $x_1x_1^{\nu}$  is the only arrow in M from  $x_1$  and  $x_2x_2^{\nu}$  is the only arrow in M from  $x_2$ .

- 3. Suppose that  $R \in \mathcal{C}[X,Z]$  (the case of  $R \in \mathcal{C}[Z,X]$  is symmetric). Note that  $\nu$  determines a bijection from  $X \times Z$  onto  $Y \times Z$ . We have to show that  $\nu$  takes the partition  $\mathcal{C}[X,Z]$  of  $X \times Z$  onto the partition  $\mathcal{C}[Y,Z]$  of  $Y \times Z$ . Let  $x_1, x_2 \in X$ ,  $y_i = x_i^{\nu}$  for i = 1, 2, and  $z_1, z_2 \in Z$ . Assuming that  $x_1 z_1 \approx x_2 z_2$ , we have to prove that  $y_1 z_1 \approx y_2 z_2$ . This follows from the fact that  $x_1 y_1$  is the only arrow in M from  $x_1$  and  $x_2 y_2$  is the only arrow in M from  $x_2$ .
- 4. The fact that  $\nu$  is a folding map from  $\mathcal{C}$  to  $\mathcal{C} \setminus X$  is a direct consequence of the three preceding parts along with the obvious observation that  $R^{\nu} = R$  for all  $R \in \mathcal{C} \setminus X$ .

$$\begin{split} R &\in \mathcal{C}[X] & \xrightarrow{f} R^f \in \mathcal{C}'[X'] \\ \downarrow^{\nu} & \downarrow^{\nu'} \\ R^{\nu} &\in \mathcal{C}[Y] & \xrightarrow{f_0} R^{\star} \in \mathcal{C}'[Y'], \quad R^{\star} = f_0(R^{\nu}) = \nu'(R^f). \end{split}$$

Figure 4: Proof of Lemma 4.4: This commutative diagram uniquely determines  $R^f$  for each  $R \in \mathcal{C}[X]$ . The similar commutative diagram holds also if  $R \in \mathcal{C}[X, Z]$  for each  $Z \neq X$  (as well as for  $R \in \mathcal{C}[Z, X]$ ).

**Lemma 4.4.** Suppose that an interspace C[X,Y] of a coherent configuration C contains a matching basis relation M. Suppose also that an interspace C'[X',Y'] of a coherent configuration C' contains a matching basis relation M'. If  $f_0$  is an algebraic isomorphism from  $C \setminus X$  to  $C' \setminus X'$  such that  $f_0(Y) = Y'$ , then  $f_0$  extends to an algebraic isomorphism f from C to C'.

*Proof.* Define a function  $\nu: V(\mathcal{C}) \to V(\mathcal{C}) \setminus X$  by  $\nu(x) = y$  for all  $xy \in M$  and  $\nu(z) = z$  for all  $z \notin X$ . A function  $\nu': V(\mathcal{C}') \to V(\mathcal{C}') \setminus X'$  is defined similarly.

Taking into account Lemma 3.3, let  $Z' = f_0(Z)$  denote the fiber of  $\mathcal{C}' \setminus X'$  corresponding to a fiber Z of  $\mathcal{C} \setminus X$  under  $f_0$ . We define a bijection  $f : \mathcal{C} \to \mathcal{C}'$  that coincides with  $f_0$  on  $\mathcal{C} \setminus X$  and bijectively maps

- C[X] onto C'[X'],
- $\mathcal{C}[X,Y] \cup \mathcal{C}[Y,X]$  onto  $\mathcal{C}'[X',Y'] \cup \mathcal{C}'[Y',X'],$
- $\mathcal{C}[X,Z] \cup \mathcal{C}[Z,X]$  onto  $\mathcal{C}'[Y',Z'] \cup \mathcal{C}'[Z',Y']$  for each  $Z \in F(\mathcal{C}), Z \neq X,Y$ .

Moreover, we require that

$$f(R^{\nu}) = (f(R))^{\nu'}. \tag{13}$$

This condition uniquely determines f because, by Parts 1–3 of Lemma 4.3, the mappings  $\nu$  and  $\nu'$  are bijective when restricted to each of the domains listed above; see Figure 4.

It is evident from the definition of f that a triple R, S, T is collocated in  $\mathcal{C}$  if and only if the triple  $R^f, S^f, T^f$  is collocated in  $\mathcal{C}'$ . If  $R, S, T \in \mathcal{C}$  are not collocated, we therefore have

$$p_{RS}^T = 0 = p_{R^f S^f}^{T^f}.$$

Assume that  $R, S, T \in \mathcal{C}$  form a collocated triple. By Part 4 of Lemma 4.3,  $\nu$  and  $\nu'$  are folding maps. According to Lemma 4.2,

$$p_{RS}^T = p_{R^{\nu}S^{\nu}}^{T^{\nu}} \tag{14}$$

and

$$p_{R^f S^f}^{T^f} = p_{\nu'(R^f)\nu'(S^f)}^{\nu'(T^f)}, \tag{15}$$

the last equality being true because  $R^f, S^f, T^f$  are collocated as well. Combining Equalities (13)–(15) and using the assumption that  $f_0$  is an algebraic isomorphism from  $\mathcal{C} \setminus X$  to  $\mathcal{C}' \setminus X'$ , we conclude that

$$p_{RS}^T = p_{R^{\nu}S^{\nu}}^{T^{\nu}} = p_{f_0(R^{\nu})f_0(S^{\nu})}^{f_0(T^{\nu})} = p_{f(R^{\nu})f(S^{\nu})}^{f(T^{\nu})} = p_{\nu'(R^f)\nu'(S^f)}^{\nu'(T^f)} = p_{R^fS^f}^{T^f}.$$

Therefore, f is an algebraic isomorphism from  $\mathcal{C}$  to  $\mathcal{C}'$ .

A function  $\nu$  in Lemma 4.3 is a kind of projection of a coherent configuration  $\mathcal{C}$  onto the smaller coherent configuration  $\mathcal{C} \setminus X$  along a matching in an interspace  $\mathcal{C}[X,Y]$ . We now consider a kind of the reverse lifting operation.

**Lemma 4.5.** Let  $\mathcal{D}$  be a coherent configuration on point set U. Let  $\mu: Y \to X$  be a bijection, where  $Y \in F(\mathcal{D})$  and  $X \cap U = \emptyset$ . Construct a rainbow  $\mathcal{C}$  on the point set  $U \cup X$  such that  $\mathcal{C}[U] = \mathcal{D}$  as follows: For each basis relation  $R \in \mathcal{D}[Y]$ , the partition  $\mathcal{C}$  of  $(U \cup X)^2$  contains

- the image  $R^{\mu} \subset X^2$  of R under  $\mu$ ;
- the relation  $\hat{R} \subset X \times Y$  defined by

$$y_1^{\mu}y_2 \in \hat{R} \iff y_1y_2 \in R;$$

• the transpose of  $\hat{R}$ .

Furthermore, for each  $Z \in F(\mathcal{D})$ ,  $Z \neq Y$ , and for each basis relation  $R \in \mathcal{D}[Y, Z]$ , the partition C contains

• the relation  $\hat{R} \subset X \times Z$  defined by

$$y^{\mu}z \in \hat{R} \iff yz \in R;$$

• the transpose of  $\hat{R}$ .

Define a map  $\nu: U \cup X \to U$  to be the inverse  $\mu^{-1}$  on X and the identity elsewhere. Then the following is true:

- **1.** C is a fibrous rainbow, and  $\nu$  is a folding map from C to D.
- **2.** C is a coherent configuration.

*Proof.* 1. The fact that C is fibrous is a straightforward consequence of the construction. It is also straightforward to see that  $\nu$  preserves the fibers and their cardinalities. Moreover, we have

- $\nu(R^{\mu}) = R$  for every  $R \in \mathcal{C}[Y]$ ;
- $\nu(\hat{R}) = R$  and  $\nu((\hat{R})^*) = R^*$  for every  $R \in \mathcal{C}[Y]$ ;

•  $\nu(\hat{R}) = R$  and  $\nu((\hat{R})^*) = R^*$  for every  $R \in \mathcal{C}[Y, Z]$ .

This shows that  $\nu$  is a folding map.

2. By Part 1 and Lemma 4.2.

**Lemma 4.6.** Suppose that an interspace C[X,Y] of a coherent configuration C contains a matching basis relation M. If C is separable, then  $C \setminus X$  is also separable.

Proof. Let  $f_0$  be an algebraic isomorphism from  $\mathcal{C}\setminus X$  to a coherent configuration  $\mathcal{D}$ . According to Lemma 3.3 and the notation introduced in Section 3.3, let  $Y' = f_0(Y)$  denote the fiber of  $\mathcal{D}$  corresponding to the fiber Y of  $\mathcal{C}$ . Fix a bijection  $\mu': Y' \to X'$ , where  $X' \cap V(\mathcal{D}) = \emptyset$ . Based on  $\mathcal{D}$  and  $\mu'$ , we construct a coherent configuration  $\mathcal{C}'$  as described in Lemma 4.5. Note that, according to this construction, the interspace  $\mathcal{C}'[X',Y']$  contains a matching basis relation, namely  $M' = \{y^{\mu'}y: y \in Y'\}$  (indeed,  $M' = \hat{D}$  for  $D = \{yy: y \in Y'\}$ ). By Lemma 4.4,  $f_0$  extends to an algebraic isomorphism f from  $\mathcal{C}$  to  $\mathcal{C}'$ . Since  $\mathcal{C}$  is separable, f is induced by a combinatorial isomorphism  $\phi: V(\mathcal{C}) \to V(\mathcal{C}')$  from  $\mathcal{C}$  to  $\mathcal{C}'$ . Denote the restriction of  $\phi$  to  $V(\mathcal{C}) \setminus X$  by  $\phi_0$ . Note that  $\phi(X) = f(X) = X'$ . Therefore, the map  $\phi_0$  is a combinatorial isomorphism from  $\mathcal{C} \setminus X$  to  $\mathcal{D}$ . Since f is induced by  $\phi$ , the algebraic isomorphism  $f_0$  is induced by the combinatorial isomorphism  $\phi_0$ .

The converse of Lemma 4.6 is known to be true due to Evdokimov and Ponomarenko [15, Lemma 9.4]. Since their proof uses a matrix language, for the reader's convenience we give an independent proof of this fact, stated as Lemma 4.8 below. Our argument is based on the following lemma, which essentially says that an algebraic isomorphism of coherent configurations preserves matching basis relations and respects projections along them.

**Lemma 4.7.** Suppose that an interspace C[X,Y] of a coherent configuration C contains a matching basis relation M. If  $f: C \to C'$  is an algebraic isomorphism of coherent configurations, then the following is true:

- **1.** M' = f(M) is a matching basis relation in the interspace C'[X', Y'], where X' = f(X) and Y' = f(Y).
- **2.** f maps bijectively
  - (a) C[X] onto C'[X'],
  - (b)  $\mathcal{C}[X,Y]$  onto  $\mathcal{C}'[X',Y']$  and  $\mathcal{C}[Y,X]$  onto  $\mathcal{C}'[Y',X']$ ,
  - (c) C[X, Z] onto C'[X', Z'] and C[Z, X] onto C'[Z', X'] for each  $Z \in F(C)$ ,  $Z \neq X, Y$ , where Z' = f(Z).
- **3.** f satisfies the condition

$$(f(R))^{\nu'} = f(R^{\nu}),$$
 (16)

where  $\nu: V(\mathcal{C}) \to V(\mathcal{C}) \setminus X$  is defined as the one-to-one map from X to Y according to M and as the identity map elsewhere, and  $\nu': V(\mathcal{C}') \to V(\mathcal{C}') \setminus X'$  is defined similarly. Thus, each of the bijections in Part 2(a)–(c) is uniquely determined by the restriction of f to  $\mathcal{C} \setminus X$ .

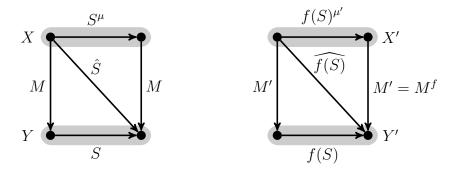


Figure 5: Proof of Lemma 4.7.

*Proof.* 1. According to the notation introduced in Section 3.3, X' and Y' are fibers of  $\mathcal{C}'$ . Note that  $R \in \mathcal{C}[X,Y]$  if and only if  $p_{RR^*}^D > 0$  for  $D = \{xx : x \in X\}$  and  $p_{R^*R}^D > 0$  for  $E = \{yy : y \in Y\}$ . Since an algebraic isomorphism preserves the intersection numbers and the pairs of mutually transposed basic relations (see [10, Proposition 2.3.18]), we conclude that

$$R \in \mathcal{C}[X,Y]$$
 if and only if  $R^f \in \mathcal{C}'[X^f,Y^f]$ . (17)

In particular, this shows that  $M' \in \mathcal{C}'[X', Y']$ . Furthermore, M' is a matching basis relation because an algebraic isomorphism preserves the valency of a basis relation (see [10, Corollary 2.3.20]).

- 2. By the general property (17) of an algebraic isomorphism.
- 3. If  $R \in \mathcal{C} \setminus X$ , then (16) is trivially true because  $\nu$  is the identity on  $\mathcal{C} \setminus X$  and  $\nu'$  is the identity on  $\mathcal{C}' \setminus X'$ . Thus, we have to consider the cases that R belongs to the cell  $\mathcal{C}[X]$  or to one of the interspaces listed in Part 2(b)–(c). Consider first the case that  $R \in \mathcal{C}[X,Y]$ . By Part 2 of Lemma 4.3,  $\nu$  takes  $\mathcal{C}[X,Y]$  bijectively onto  $\mathcal{C}[Y]$  and, similarly,  $\nu'$  takes  $\mathcal{C}'[X',Y']$  bijectively onto  $\mathcal{C}[Y']$ . Given  $S \in \mathcal{C}[Y]$ , let  $\hat{S}$  denote the basis relation in  $\mathcal{C}[X,Y]$  such that  $(\hat{S})^{\nu} = S$ . The similar notation will be used also for  $\mathcal{C}'$ . Since  $\widehat{R}^{\nu} = R$  for every  $R \in \mathcal{C}[X,Y]$  (and similarly in  $\mathcal{C}'$ ), we actually have to prove that

$$f(\hat{S}) = \widehat{f(S)} \tag{18}$$

for any  $S \in \mathcal{C}[Y]$ . Note that  $T = \hat{S}$  if and only if  $p_{MS}^T = 1$ ; see Figure 5. Similarly,  $T' = \widehat{f(S)}$  if and only if  $p_{M'f(S)}^{T'} = 1$ . This implies Equality (18) as

$$p_{M'f(S)}^{f(\hat{S})} = p_{f(M)f(S)}^{f(\hat{S})} = p_{MS}^{\hat{S}} = 1.$$

Suppose now that  $R \in \mathcal{C}[X]$ . By Part 1 of Lemma 4.3,  $\nu$  takes  $\mathcal{C}[X]$  bijectively onto  $\mathcal{C}[Y]$ , and similarly  $\nu'$  takes  $\mathcal{C}'[X']$  bijectively onto  $\mathcal{C}'[Y']$ . Let  $\mu: Y \to X$  be the inverse of  $\nu$  and, similarly,  $\mu': Y' \to X'$  be the inverse of  $\nu'$ . Now we have to prove that

$$f(S^{\mu}) = f(S)^{\mu'} \tag{19}$$

for any  $S \in \mathcal{C}[Y]$ . Note that  $T = S^{\mu}$  if and only if  $p_{TM}^{\hat{S}} = 1$ . Similarly,  $T' = f(S)^{\mu'}$  if and only if  $p_{T'M'}^{\widehat{f(S)}} = 1$ . Using (18), this implies Equality (19) as

$$p_{f(S^{\mu})M'}^{\widehat{f(S)}} = p_{f(S^{\mu})f(M)}^{f(\hat{S})} = p_{S^{\mu}M}^{\hat{S}} = 1.$$

The other cases are handled similarly.

**Lemma 4.8.** Suppose that an interspace C[X,Y] of a coherent configuration C contains a matching basis relation. If  $C \setminus X$  is separable, then C is separable too.

*Proof.* Let f be an algebraic isomorphism from  $\mathcal{C}$  to  $\mathcal{C}'$ . Let X' = f(X) be the fiber of  $\mathcal{C}'$  corresponding to the fiber X of  $\mathcal{C}$ . Denote the restriction of f to  $\mathcal{C} \setminus X$  by  $f_0$ . By Lemma 3.5,  $f_0$  is an algebraic isomorphism from  $\mathcal{C} \setminus X$  to  $\mathcal{C}' \setminus X'$ . By the assumption that  $\mathcal{C} \setminus X$  is separable,  $f_0$  is induced by a combinatorial isomorphism  $\phi_0: V(\mathcal{C}) \setminus X \to V(\mathcal{C}') \setminus X'$ .

Let Y' = f(Y). By Part 1 of Lemma 4.7, the basis relation  $M' = M^f$  is a matching in the interspace  $\mathcal{C}'[X',Y']$ . Define a bijection  $\nu: X \to Y$ , as usually, by  $\nu(x) = y$  for all  $xy \in M$  and a bijection  $\nu': X' \to Y'$  similarly. Let us extend  $\phi_0$  to a bijection  $\phi: V(\mathcal{C}) \to V(\mathcal{C}')$  by setting

$$\phi = (\nu')^{-1} \circ \phi_0 \circ \nu$$

on X, that is, requiring the diagram

$$\begin{array}{ccc}
X & \xrightarrow{\phi} & X' \\
\downarrow^{\nu} & & \downarrow^{\nu'} \\
Y & \xrightarrow{\phi_0} & Y'
\end{array}$$

be commutative.

Extend  $\nu$  to the whole point set  $V(\mathcal{C})$  by the identity on  $V(\mathcal{C}) \setminus X$  and, similarly, extend  $\nu'$  to  $V(\mathcal{C}')$  by the identity on  $V(\mathcal{C}') \setminus X'$ . Recall the properties of  $\nu$  and  $\nu'$  established in Parts 1–3 of Lemma 4.3. The definition of  $\phi$  implies that

$$\phi \circ \nu = \nu' \circ \phi.$$

It follows that

$$\phi(R)^{\nu'} = \phi(R^{\nu})$$

for every basis relation  $R \in \mathcal{C}$ . Comparing this with Equality (16) in Lemma 4.7, we see that  $f(R) = \phi(R)$  for all  $R \in \mathcal{C}$  as a consequence of Parts 2–3 of this lemma. We conclude that f is induced by  $\phi$ .

Thus, the proof of Lemma 4.1 is complete.

Corollary 4.9 (cf. [10, Exercise 3.7.20]). Every coherent configuration  $\mathcal{D}$  with maximum fiber size at most 3 is separable.

Proof. By Lemma 3.1,  $\mathcal{D}$  decomposes in a direct sum of indecomposable coherent configurations each with fibers of the same size which can be 3, or 2, or 1. An indecomposable coherent configuration with maximum fibers size 1 is actually a single-point configuration and, hence, is separable. Let  $s \in \{2,3\}$  and suppose that  $\mathcal{C}$  is an indecomposable coherent configuration with all fibers of the same size s. As it is seen from Figure 2, every non-uniform interspace of  $\mathcal{C}$  contains a matching basis relation. Lemma 4.1 reduces deciding separability of a  $\mathcal{C}$  to deciding separability of a smaller coherent configuration. Applying this reduction repeatedly, we see that  $\mathcal{C}$  is separable if and only if the association scheme  $\mathcal{C}[X]$  for the only remaining fiber X is separable. The 2- and 3-point association schemes are shown in Figure 1; all of them are separable. Therefore,  $\mathcal{C}$  is separable. By Lemma 3.2, we conclude that  $\mathcal{D}$  is separable.

Note that Corollary 4.9, along with Theorem 2.5, implies the Immerman-Lander result [25] that every graph of color multiplicity at most 3 is amenable.

# 5 Cutting it down: 2-Point fibers

Corollary 4.9, along with Lemmas 3.2 and 3.1, reduces deciding whether a coherent configuration  $\mathcal{C}$  with maximum fiber size 4 is separable to the case that  $\mathcal{C}$  has fibers only of size 4 or 2. By Lemma 4.1, we can also assume that no interspace of  $\mathcal{C}$  contains a matching basis relation. The following lemma makes further reduction.

**Lemma 5.1.** Let C be an indecomposable coherent configuration on more than 2 points with fibers only of size 4 or 2. Suppose that no interspace of C contains a matching basis relation. Let  $X \in F(C)$  with |X| = 2. Under these conditions, C is separable if and only if  $C \setminus X$  is separable.

We remark that Lemma 5.1 is applicable to the multipede graphs of color multiplicity at most 4 (see Section 1 and Remark 9.4). In this setting, Neuen and Schweitzer [32, Section 4.2] use the operation of removing vertex color classes of size 2 in order to reduce the number of vertices in their construction of benchmark graphs challenging for practical isomorphism solvers.

To prove Lemma 5.1, we first collect some structural information.

# 5.1 Direct and skewed connections of interspaces

We use the notation introduced in Section 3.1; see, in particular, Figure 3.

#### Lemma 5.2.

- **1.** Suppose that  $C[X,Y] \simeq 2K_{1,2}$ . If C[X,Y] contains a relation  $R = \{x_1y_1, x_1y_2, x_2y_3, x_2y_4\}$ , then C[Y] contains a basis relation  $S = \{y_1y_2, y_2y_1, y_3y_4, y_4y_3\}$ .
- **2.** Suppose that  $C[X,Y] \simeq 2K_{2,2}$ . If C[X,Y] contains a relation  $R = \{x_1, x_2\} \times \{y_1, y_2\} \cup \{x_3, x_4\} \times \{y_3, y_4\}$ , then C[Y] contains a basis relation  $S = \{y_1y_2, y_2y_1, y_3y_4, y_4y_3\}$ .

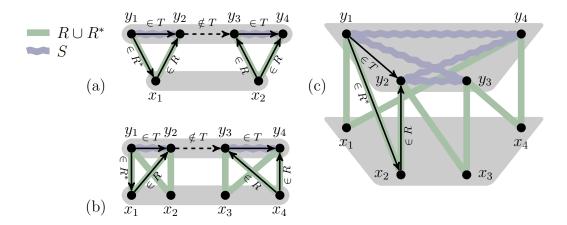


Figure 6: Proof of Lemma 5.2: (a) Part 1; (b) Part 2; (c) Part 3.

- **3.** Suppose that  $C[X,Y] \simeq C_8$ . If C[X,Y] contains a relation  $R = \{x_1y_1, x_2y_1, x_2y_2, x_3y_2, x_3y_3, x_4y_3, x_4y_4, x_1y_4\}$ , then  $C[Y] \simeq C_4$  and  $S = \{y_1y_3, y_3y_1, y_2y_4, y_4y_2\}$  is one of the two irreflexive basis relations of C[Y].
- Proof. 1. Let T be the basis relation of C[Y] containing the arrow  $y_1y_2$ . We have  $T \subseteq S$  because  $p_{R^*R}^T > 0$ . For example,  $y_2y_3 \notin T$  because  $y_1y_2$  extends to  $y_1x_1y_2$  and  $y_2y_3$  cannot be extended to a triangle of this kind. On the other hand,  $S \subseteq T$  because  $p_{RT}^R > 0$ . For example,  $y_3y_4 \in T$  because otherwise, while  $x_1y_2$  extends to  $x_1y_1y_2$ , the pair  $x_2y_4$  could not be extended to a triangle of this kind; see Figure 6(a).
- 2. Literally the same argument (but with  $x_4y_4$  instead of  $x_2y_4$ ) applies also for this part; see Figure 6(b).
- 3. Again, let T be the basis relation containing the arrow  $y_1y_2$ . We have  $T \cap S = \emptyset$  because  $p_{R^*R}^T > 0$ . Furthermore,  $p_{RT}^R > 0$ , and this implies that T is exactly the irreflexive complement of S in  $Y^2$ ; see Figure 6(c).

The following definitions play an important role not only in the proof of Lemma 5.1 but also in the subsequent sections. In the context of Lemma 5.2, we say that C[X,Y] determines a matching basis relation in C[Y] (namely  $\{y_1y_2, y_2y_1, y_3y_4, y_4y_3\}$  in Parts 1–2 and  $\{y_1y_3, y_3y_1, y_2y_4, y_4y_2\}$  in Part 3). Suppose that C[X,Y] determines a matching M in Y, and C[Z,Y] determines a matching M' in Y. We say that C[X,Y] and C[Z,Y] have a direct connection at Y if M=M'. If  $M \neq M'$ , we say that C[X,Y] and C[Z,Y] have a skewed connection at Y (or are, respectively, directly or askew connected at Y).

We conclude this subsection with a lemma that provides an important information on the structure of matching-free coherent configurations.

**Lemma 5.3** (Transitivity of direct  $2K_{2,2}$ -connections). If  $C[X,Y] \simeq 2K_{2,2}$  and  $C[Z,Y] \simeq 2K_{2,2}$  are directly connected at Y, then either C[X,Z] contains a matching basis relation or  $C[X,Z] \simeq 2K_{2,2}$  and the connections between C[Z,X] and C[Y,X] at X and between C[X,Z] and C[Y,Z] at Z are direct.

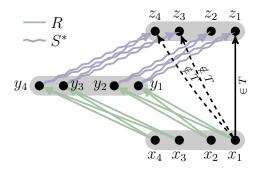


Figure 7: Proof of Lemma 5.3.

*Proof.* Fix basis relations  $R \in \mathcal{C}[X,Y]$  and  $S \in \mathcal{C}[Z,Y]$ . By assumption, they determine the same matching in  $\mathcal{C}[Y]$ . Specifically, let

$$R = \{x_1, x_2\} \times \{y_1, y_2\} \cup \{x_3, x_4\} \times \{y_3, y_4\}$$

and

$$S = \{z_1, z_2\} \times \{y_1, y_2\} \cup \{z_3, z_4\} \times \{y_3, y_4\};$$

see Figure 7. Let  $T \in \mathcal{C}[X,Z]$  be the basis relation containing the arrow  $x_1z_1$ . Note that  $p_{RS^*}^T = 2$ . This equality implies that T contains neither  $x_1z_3$  nor  $x_1z_4$ . Therefore, the valency of T is either 1 or 2. In the former case T is a matching basis relation. Suppose that d(T) = 2 and, hence,  $x_1z_2 \in T$ . It remains to exclude the possibility that T is of  $C_8$ -type.

Using the fact that  $z_2x_1 \in T^*$  and repeating the same argument as above, we conclude that also  $z_2x_2 \in T^*$ . This yields  $x_2z_2 \in T$  and, repeating the same argument, we also derive  $x_2z_1 \in T$ . It follows that T contains the set  $\{x_1, x_2\} \times \{z_1, z_2\}$  and, hence, is of  $2K_{2,2}$ -type.

Finally, note that T and  $S^*$  determine the same matching in  $\mathcal{C}[Z]$  and that  $T^*$  and  $R^*$  determine the same matching in  $\mathcal{C}[X]$ .

# **5.2** Subconfigurations $C[X \cup Y \cup Z]$ with $C[X,Y] \simeq 2K_{1,2}$

**Lemma 5.4.** Let  $X, Y, Z \in F(\mathcal{C})$  with |X| = 2 and |Y| = |Z| = 4. Suppose that  $\mathcal{C}[X, Y] \simeq 2K_{1,2}$ .

- **1.** If  $C[Z,Y] \simeq 2K_{2,2}$  with direct connection to C[X,Y] at Y, then  $C[X,Z] \simeq 2K_{1,2}$  with direct connection to C[Y,Z] at Z.
- **2.** If  $C[Z,Y] \simeq 2K_{2,2}$  with skewed connection to C[X,Y] at Y, then C[X,Z] is uniform.
- **3.** If  $C[Z,Y] \simeq C_8$ , then C[X,Z] is uniform.
- **4.** If C[Z,Y] is uniform, then C[X,Z] is uniform too.

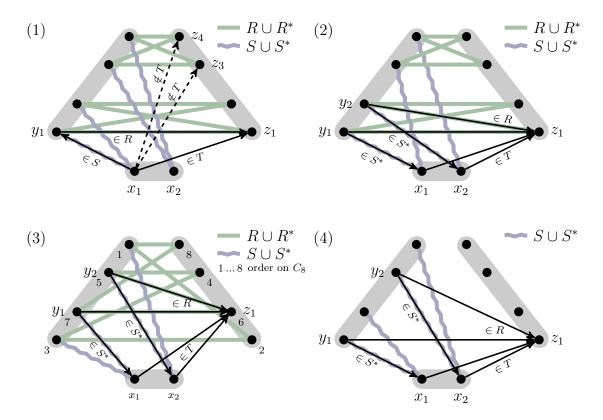


Figure 8: Proof of Lemma 5.4. An auxiliary enumeration of the points in  $Y \cup Z$  corresponds to the 8-cycle underlying the basis relation R in Part 3.

*Proof.* Fix a basis relation  $S \in \mathcal{C}[X,Y]$ . Also, fix a basis relation  $R \in \mathcal{C}[Y,Z]$ ; Figure 8 gives the corresponding picture for each part of the lemma. We will refer to the points of  $\mathcal{C}[X \cup Y \cup Z]$  using these pictures.

- 1. Let T be the basis relation of C[X, Z] containing the arrow  $x_1z_1$ . It suffices to show that neither  $x_1z_3$  nor  $x_1z_4$  is in T. This follows from the fact that  $p_{SR}^T > 0$ .
- 2. It suffices to prove that all the arrows from  $z_1$  to X, i.e.,  $z_1x_1$  and  $z_1x_2$ , are in the same basis relation. We will prove that the transposed arrows  $x_1z_1$  and  $x_2z_1$  are in the same basis relation. Denote the basis relation containing  $x_1z_1$  by T. Looking at the triple  $y_1x_1z_1$ , we see that  $p_{S^*T}^R > 0$ . Since  $y_2z_1 \in R$  and  $x = x_2$  is the only point such that  $y_2x \in S^*$ , we conclude that  $x_2z_1 \in T$ .
- 3. By Parts 1 and 3 of Lemma 5.2, each of the interspaces C[X, Y] and C[Z, Y] determines a matching basis relation in the cell C[Y]. Moreover, Part 3 of Lemma 5.2 implies that C[Y] contains a unique matching relation. Therefore, the connection of C[X, Y] and C[Z, Y] at Y is exactly as shown in Figure 8. The rest of the proof is literally the same as in the preceding part, even though the points  $y_1$ ,  $y_2$ , and  $z_1$  now have a different position, as shown in Figure 8(3).
- 4. The proof is literally the same as in Part 2, where the new position of the points  $y_1$ ,  $y_2$  is shown in Figure 8(4).

### 5.3 Proof of Lemma 5.1

Since  $\mathcal{C}$  is indecomposable, it contains a non-uniform interspace  $\mathcal{C}[X,Y]$ . It is impossible that |Y|=2 because then  $\mathcal{C}[X,Y]$  would contain a matching; see Figure 2. It follows that |Y|=4. We conclude that  $\mathcal{C}[X,Y]\simeq 2K_{1,2}$ , as this is the only, up to isomorphism, non-uniform interspace between two fibers of sizes 2 and 4; see Figure 3.

To be specific, let  $X = \{x_1, x_2\}$  and  $Y = \{y_1, y_2, y_3, y_4\}$ , and suppose that  $\mathcal{C}[X, Y]$  consists of the relation

$$T = \{x_1\} \times \{y_1, y_2\} \cup \{x_2\} \times \{y_3, y_4\}$$
 (20)

and its complement  $X \times Y \setminus T$ . We now proceed to proving that  $\mathcal{C}$  is separable if and only if  $\mathcal{C} \setminus X$  is separable.

 $(\Longrightarrow)$  Let  $f_0$  be an algebraic isomorphism from  $\mathcal{C}\setminus X$  to a coherent configuration  $\mathcal{D}$ . It suffices to extend  $\mathcal{D}$  to a coherent configuration  $\mathcal{C}'$  such that  $f_0$  extends to an algebraic isomorphism f from  $\mathcal{C}$  to  $\mathcal{C}'$ . Indeed, since  $\mathcal{C}$  is separable, such an f is induced by a combinatorial isomorphism  $\phi: V(\mathcal{C}) \to V(\mathcal{C}')$ , and the restriction of  $\phi$  to  $V(\mathcal{C}) \setminus X$  will give us a combinatorial isomorphism from  $\mathcal{C} \setminus X$  to  $\mathcal{D}$  inducing  $f_0$ .

We construct  $\mathcal{C}'$  and f as follows. First of all, take  $X' = \{x'_1, x'_2\}$  such that  $X' \cap V(\mathcal{D}) = \emptyset$ . This will be a fiber of  $\mathcal{C}'$ . The 2-point association scheme  $\mathcal{C}'[X']$  is unique. The map f is defined on the two basis relations of the cell  $\mathcal{C}[X]$  uniquely in an obvious way: It maps the (ir)reflexive relation of  $\mathcal{C}[X]$  to the (ir)reflexive relation of  $\mathcal{C}'[X']$ .

Let  $Y' = f_0(Y)$  denote the fiber of  $\mathcal{D}$  corresponding to the fiber Y of  $\mathcal{C} \setminus X$  under  $f_0$ . It follows from (20) by Part 1 of Lemma 5.2, that  $\mathcal{C}[X,Y]$  determines the matching basis relation

$$M = \{y_1 y_2, y_2 y_1, y_3 y_4, y_4 y_3\}$$
 (21)

in C[Y]. Note that  $M' = f_0(M)$  is a matching basis relation in C'[Y'] (cf. the proof of Part 1 of Lemma 4.7). To be specific, let  $Y' = \{y'_1, y'_2, y'_3, y'_4\}$  and

$$M' = \{y_1'y_2', y_2'y_1', y_3'y_4', y_4'y_3'\}.$$

We set the interspace  $\mathcal{C}'[X',Y']$  to be the partition of  $X'\times Y'$  into the relations

$$T' = \{x_1'\} \times \{y_1', y_2'\} \cup \{x_2'\} \times \{y_3', y_4'\}$$

and  $X' \times Y' \setminus T'$ . Furthermore, we set f(T) = T' and  $f(X \times Y \setminus T) = X' \times Y' \setminus T'$ . This will define f also on  $\mathcal{C}[Y,X]$  according to the general property  $f(R^*) = f(R)^*$  of an algebraic isomorphism. Note that the extension f, as defined so far, is an algebraic isomorphism from  $\mathcal{C}[X \cup Y]$  to the current fragment  $\mathcal{C}'[X' \cup Y']$  of  $\mathcal{C}'$ .

Given  $Z \in F(\mathcal{C} \setminus X)$ , let  $Z' = f_0(Z)$ . It remains, for each  $Z \neq Y$ , to construct  $\mathcal{C}'[X', Z']$  and to define f locally as a bijection from  $\mathcal{C}[X, Z]$  to  $\mathcal{C}'[X', Z']$ . If  $\mathcal{C}[X, Z]$  is uniform, which is always the case when |Z| = 2, we set  $\mathcal{C}'[X', Z']$  also to be uniform, and correspondingly define  $f(X \times Z) = X' \times Z'$ . Assume now that  $\mathcal{C}[X, Z]$  is non-uniform and, hence, |Z| = 4 and  $\mathcal{C}[X, Z] \simeq 2K_{1,2}$ .

In this case, Lemma 5.4 implies that  $\mathcal{C}[Z,Y] \simeq 2K_{2,2}$  and that this interspace is directly connected to  $\mathcal{C}[X,Y]$  at Y. Fix a basis relation  $S_Z \in \mathcal{C}[Z,Y]$ . Fix an enumeration  $z_1, z_2, z_3, z_4$  of the points of Z such that

$$S_Z = \{z_1, z_2\} \times \{y_1, y_2\} \cup \{z_3, z_4\} \times \{y_3, y_4\}. \tag{22}$$

Since  $f_0$  is an algebraic isomorphism from  $\mathcal{C} \setminus X$  to  $\mathcal{D}$ , we have  $\mathcal{D}[Z', Y'] \simeq 2K_{2,2}$ , and this interspace determines the matching M' in  $\mathcal{D}[Y']$ . Therefore, the points of Z' can be enumerated so that

$$f_0(S_Z) = \{z_1', z_2'\} \times \{y_1', y_2'\} \cup \{z_3', z_4'\} \times \{y_3', y_4'\}, \tag{23}$$

and we fix such an enumeration  $z'_1, z'_2, z'_3, z'_4$ . Part 1 of Lemma 5.4 implies that  $\mathcal{C}[X, Z]$  is directly connected to  $\mathcal{C}[Y, Z]$  at Z and, therefore, consists of the relation

$$R_Z = \{x_1\} \times \{z_1, z_2\} \cup \{x_2\} \times \{z_3, z_4\}$$
 (24)

and its complement  $X \times Z \setminus R_Z$ . We, therefore, define the interspace  $\mathcal{C}'[X', Z'] \simeq 2K_{1,2}$  by requiring that it determines the matching  $\{z'_1z'_2, z'_2z'_1, z'_3z'_4, z'_4z'_3\}$  in  $\mathcal{C}'[Z']$ . This condition defines  $\mathcal{C}'[X', Z']$  uniquely and ensures that  $\mathcal{C}'[X' \cup Y' \cup Z']$  is a coherent configuration. There still remain two different possibilities to define f on  $\mathcal{C}[X, Z]$ . Our choice is this: We set

$$f(R_Z) = \{x_1'\} \times \{z_1', z_2'\} \cup \{x_2'\} \times \{z_3', z_4'\}. \tag{25}$$

Note that the basis relation  $R_Z$  is chosen in (24) in such a way that the set  $T \cup T^* \cup S_Z \cup S_Z^* \cup R_Z \cup R_Z^*$ , seen as a symmetric irreflexive relation, forms a graph with two connected components, one containing  $x_1$  and the other containing  $x_2$ . Likewise, the basis relation  $f(R_Z)$  is defined by (25) so that  $T' \cup (T')^* \cup f(S_Z) \cup f(S_Z)^* \cup f(R_Z) \cup f(R_Z)^*$  also has two connected components. This ensures that f is an algebraic isomorphism from  $C[X \cup Y \cup Z]$  to  $C'[X' \cup Y' \cup Z']$ , see Figure 9.

The construction of  $\mathcal{C}'$  and  $f: \mathcal{C} \to \mathcal{C}'$  is complete. It remains to argue that  $\mathcal{C}'$  is indeed a coherent configuration and that f is an algebraic isomorphism from  $\mathcal{C}$  to  $\mathcal{C}'$ . For this purpose, we use Lemma 3.4.

Let us check that the assumptions of Lemma 3.4 are fulfilled. They are trivially true if A, B, C are fibers of  $C \setminus X$ . We, therefore, assume that C = X. The case that  $Y \in \{A, B\}$  is already treated above. Thus, it remains to consider subconfigurations  $C[X \cup A \cup B]$  for each pair  $A, B \in F(C)$  such that  $A \neq B$  and neither A nor B is in  $\{X, Y\}$ . Fix such a pair A, B. We will prove a stronger fact: There is a bijection  $\phi = \phi_{AB}$  from  $X \cup A \cup B$  onto  $X' \cup A' \cup B'$  that is a combinatorial isomorphism from  $C[X \cup A \cup B]$  to  $C'[X' \cup A' \cup B']$  and that induces the restriction of f to  $C[X \cup A \cup B]$ .

The restriction of  $f_0$  to  $\mathcal{C}[A \cup B]$  is an algebraic isomorphism from  $\mathcal{C}[A \cup B]$  to  $\mathcal{C}'[A' \cup B']$ . It is easy to deduce from Lemma 5.2 that this algebraic isomorphism is induced by a combinatorial isomorphism  $\phi_0: A \cup B \to A' \cup B'$ . We will take  $\phi$  to be an extension of  $\phi_0$  to a bijection from  $X \cup A \cup B$  to  $X' \cup A' \cup B'$ . Note that  $\phi$  can be defined on X in two ways. In both cases, this will be a combinatorial isomorphism

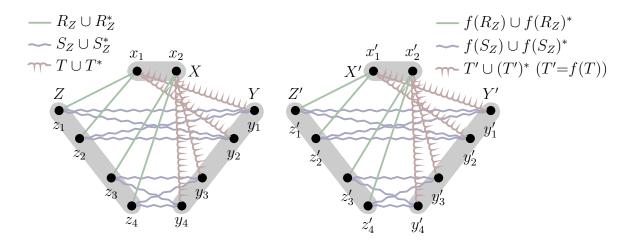


Figure 9: Proof of Lemma 5.1: Defining the algebraic isomorphism f locally from  $\mathcal{C}[X \cup Y \cup Z]$  to  $\mathcal{C}[X' \cup Y' \cup Z']$ .

from  $C[X \cup A \cup B]$  to  $C'[X' \cup A' \cup B']$ . We only need to ensure that  $\phi$  induces f. To define  $\phi$ , we consider three cases.

Case 1: Both C[A, X] and C[B, X] are uniform. In this case,  $\phi(X \times Z) = X' \times Z' = f(X \times Z)$  for both  $Z \in \{A, B\}$  independently of how  $\phi$  is defined on X.

Case 2: Exactly one of the interspaces C[A, X] and C[B, X], say C[A, X], is non-uniform. Note that  $C[X, A] \simeq 2K_{1,2}$ . Let  $a_1, a_2, a_3, a_4$  be the enumeration of A and  $a'_1, a'_2, a'_3, a'_4$  be the enumeration of A' fixed in the course of our construction of C'; cf. (22) and (23). Let

$$M_A = \{a_1 a_2, a_2 a_1, a_3 a_4, a_4 a_3\} \tag{26}$$

and

$$M_A' = \{a_1'a_2', a_2'a_1', a_3'a_4', a_4'a_3'\}$$
(27)

be the matchings determined by the interspaces C[Y, A] in the cell C[A] and C'[Y', A'] in C'[A']. Equalities (22) and (23) applied to Z = A show that  $f_0(M_A) = M'_A$ . It follows that either

$$\phi_0(\{a_1, a_2\}) = \{a'_1, a'_2\} \text{ and } \phi_0(\{a_3, a_4\}) = \{a'_3, a'_4\}$$

or

$$\phi_0(\{a_1, a_2\}) = \{a_3', a_4'\} \text{ and } \phi_0(\{a_3, a_4\}) = \{a_1', a_2'\}.$$

In the former case, we extend  $\phi_0$  to  $\phi$  by  $\phi(x_i) = x_i'$  for both i = 1, 2. In the latter case, we have to swap the values of  $\phi$  on X by setting  $\phi(x_1) = x_2'$  and  $\phi(x_2) = x_1'$ . By Equalities (24) and (25) applied to Z = A, this ensures that  $\phi(R_A) = f(R_A)$  and, therefore, f on  $\mathcal{C}[A \cup B \cup X]$  is induced by  $\phi$ .

Case 3: Both C[A, X] and C[B, X] are non-uniform. Thus,  $C[X, A] \simeq 2K_{1,2}$  and  $C[X, B] \simeq 2K_{1,2}$ . Like in the preceding case, let  $a_1, a_2, a_3, a_4$  and  $a'_1, a'_2, a'_3, a'_4$  be the enumerations of A and A' that were fixed in the course of our construction of C'. Similarly, let  $b_1, b_2, b_3, b_4$  and  $b'_1, b'_2, b'_3, b'_4$  be the enumerations of B and B'. Since the

basis relations  $S_A$  and  $S_B$  (fixed in the course of our construction of  $\mathcal{C}'$ ) are directly connected at  $\mathcal{C}[Y]$ , Lemma 5.3 implies that the interspace  $\mathcal{C}[A, B]$  consists of the basis relation

$$Q_{AB} = \{a_1, a_2\} \times \{b_1, b_2\} \cup \{a_3, a_4\} \times \{b_3, b_4\}$$

and its complement  $A \times B \setminus Q_{AB}$ . Since the graph  $Q_{AB} \cup Q_{AB}^* \cup S_A \cup S_A^* \cup S_B \cup S_B^*$  has two connected components, the graph  $f_0(Q_{AB}) \cup f_0(Q_{AB})^* \cup f_0(S_A) \cup f_0(S_A)^* \cup f_0(S_B)^*$  must also have two connected components, which implies that

$$f_0(Q_{AB}) = \{a'_1, a'_2\} \times \{b'_1, b'_2\} \cup \{a'_3, a'_4\} \times \{b'_3, b'_4\}.$$

Using the fact that the coherent configuration  $C[A \cup B \cup Y]$  has three  $2K_{2,2}$ -interspaces that are pairwise directly connected, we see that the restriction of  $f_0$  to an algebraic isomorphism from  $C[A \cup B \cup Y]$  to  $C'[A' \cup B' \cup Y']$  is induced by a combinatorial isomorphism  $\phi_0$  (now  $\phi_0$  is defined on a larger domain than  $A \cup B$ ). Since  $\phi_0(Q_{AB}) = f_0(Q_{AB})$ , we have either

$$\phi_0(\{a_1, a_2\}) = \{a_1', a_2'\} \text{ and } \phi_0(\{b_1, b_2\}) = \{b_1', b_2'\}$$
(28)

or

$$\phi_0(\{a_1, a_2\}) = \{a_3', a_4'\} \text{ and } \phi_0(\{b_1, b_2\}) = \{b_3', b_4'\}.$$

The coherent configuration  $C[A \cup B \cup Y]$  has a combinatorial automorphism that maps each basis relation onto itself and swaps the sets  $\{a_1, a_2\}$  and  $\{a_3, a_4\}$  and simultaneously the sets  $\{b_1, b_2\}$  and  $\{b_3, b_4\}$ . Applying this automorphism if necessary, we can modify  $\phi_0$  and ensure Equality (28). Now, extending  $\phi_0$  to  $\phi$  by  $\phi(x_i) = x_i'$  for each i = 1, 2, we see that

$$\phi(R_A) = f(R_A)$$
 and  $\phi(R_B) = f(R_B)$ 

for the basis relations  $R_A$  and  $R_B$  introduced by (24); see (25). It follows that  $\phi$  induces f on  $\mathcal{C}[A \cup B \cup X]$ , as desired.

( $\iff$ ) Let f be an algebraic isomorphism from  $\mathcal{C}$  to a coherent configuration  $\mathcal{C}'$ . For each fiber  $A \in F(\mathcal{C})$ , let A' = f(A) denote the corresponding fiber of  $\mathcal{C}'$ . Denote the restriction of f to  $\mathcal{C} \setminus X$  by  $f_0$  and note that  $f_0$  is an algebraic isomorphism from  $\mathcal{C} \setminus X$  to the coherent configuration  $\mathcal{C}' \setminus X'$ . Since  $\mathcal{C} \setminus X$  is separable,  $f_0$  is induced by a combinatorial isomorphism  $\phi_0 : V(\mathcal{C}) \setminus X \to V(\mathcal{C}') \setminus X'$ . Extend  $\phi_0$  to a map  $\phi : V(\mathcal{C}) \to V(\mathcal{C}')$  as follows. We use the enumeration  $x_1, x_2$  of X and  $y_1, y_2, y_3, y_4$  of Y fixed in the beginning of the proof. Recall that the interspace  $\mathcal{C}[X, Y]$  consists of the relation T specified by (20). Denote  $y'_i = \phi_0(y_i)$  for each  $i \leq 4$ . Number the points  $x'_1$  and  $x'_2$  of X' so that

$$f(T) = \{x_1'\} \times \{y_1', y_2'\} \cup \{x_2'\} \times \{y_3', y_4'\}. \tag{29}$$

Now, we set  $\phi(x_1) = x_1'$  and  $\phi(x_2) = x_2'$ . The bijection  $\phi$  is therewith defined and we have to show that  $\phi$  is a combinatorial isomorphism from  $\mathcal{C}$  to  $\mathcal{C}'$  inducing the algebraic isomorphism f. It suffices to do this locally for subconfigurations  $\mathcal{C}[X \cup Z]$ 

and  $\mathcal{C}'[X' \cup Z']$ , for each  $Z \in F(\mathcal{C} \setminus X)$ . Since |X| = 2, the restriction of  $\phi$  to  $X \cup Z$  is a combinatorial isomorphism from  $\mathcal{C}[X \cup Z]$  to  $\mathcal{C}'[X' \cup Z']$  even irrespectively of how  $\phi$  is defined on X. Thus, we only have to prove that  $\phi$  induces the restriction of f to  $\mathcal{C}[X \cup Z]$ . Our definition of  $\phi$  ensures this for Z = Y, as it immediately follows from (20) and (29).

Suppose that  $Z \neq Y$ . If  $\mathcal{C}[X, Z]$  is uniform, we have nothing to prove. Assume, therefore, that  $\mathcal{C}[X, Z]$  is non-uniform. Recall that  $\mathcal{C}[X, Z] \simeq 2K_{1,2}$  and  $\mathcal{C}[Z, Y] \simeq 2K_{2,2}$ . We refer to the enumeration  $z_1, z_2, z_3, z_4$  we have fixed for each such Z. Denote  $z'_i = \phi_0(z_i)$ . Consider the basis relation

$$S_Z = \{z_1, z_2\} \times \{y_1, y_2\} \cup \{z_3, z_4\} \times \{y_3, y_4\}$$

as in (22). Since  $f_0$  is induced by  $\phi_0$ , we have

$$f(S_Z) = \{z_1', z_2'\} \times \{y_1', y_2'\} \cup \{z_3', z_4'\} \times \{y_3', y_4'\}. \tag{30}$$

Consider now the basis relation

$$R_Z = \{x_1\} \times \{z_1, z_2\} \cup \{x_2\} \times \{z_3, z_4\}$$

in C[X, Z] specified by (24). Since f provides an algebraic isomorphism from  $C[X \cup Y \cup Z]$  to  $C'[X' \cup Y' \cup Z']$ , Equalities (29) and (30) readily imply that

$$f(R_Z) = \{x_1'\} \times \{z_1', z_2'\} \cup \{x_2'\} \times \{z_3', z_4'\}.$$

Thus,  $f(R_Z) = \phi(R_Z)$ , and f is induced by  $\phi$  on  $\mathcal{C}[X, Z]$  and, hence, everywhere. The proof of Lemma 5.1 is complete.

# 6 Cutting it down: Interspaces with an 8-cycle

Taking into account Lemma 5.1, our task now reduces to deciding separability of a coherent configuration C under the following three conditions:

- (1)  $\mathcal{C}$  is indecomposable;
- (2) all fibers of C have size exactly 4;
- (3) the interspaces of  $\mathcal{C}$  do not contain any matching basis relation.

Our next step is excluding  $C_8$ -interspaces. For  $X, Y \in F(\mathcal{C})$ , we denote  $\mathcal{C} \setminus X, Y = \mathcal{C}[V(\mathcal{C}) \setminus (X \cup Y)]$ .

**Lemma 6.1.** Let C be a coherent configuration satisfying Conditions (1)–(3) above. Suppose that C has at least three fibers and that there is a  $C_8$ -interspace C[X,Y]. Under these conditions, C is separable if and only if  $C \setminus X, Y$  is separable.

To prove Lemma 6.1, we need further structural information.

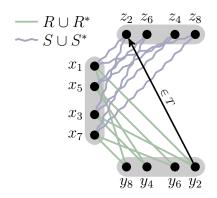


Figure 10: Proof of Lemma 6.2.

## 6.1 Isolation of $C_8$ -interspaces

The following lemma shows that in a matching-free coherent configuration no two  $C_8$ -interspaces can share a fiber.

**Lemma 6.2.** If  $C[X,Y] \simeq C_8$  and  $C[X,Z] \simeq C_8$ , then the interspace C[Y,Z] contains a matching basis relation.

Proof. Fix basis relations  $R \in \mathcal{C}[Y,X]$  and  $S \in \mathcal{C}[X,Z]$ . Let  $X = \{x_1, x_3, x_5, x_7\}$ ,  $Y = \{y_2, y_4, y_6, y_8\}$ , and  $Z = \{z_2, z_4, z_6, z_8\}$ , where the points are indexed according to the 8-cycles underlying R and S; see Figure 10. Let  $T \in \mathcal{C}[Y,Z]$  be the basis relation containing the arrow  $y_2z_2$ . Note that  $p_{RS}^T = 2$ . This equality prevents the membership in T of the other arrows  $y_2z_4$ ,  $y_2z_6$ , and  $y_2z_8$  from  $y_2$  to Z. It follows that T has valency 1, that is, it is a matching basis relation.

#### 6.2 Proof of Lemma 6.1

Since  $\mathcal{C}$  is indecomposable, X or Y is connected by a non-uniform interspace to a fiber U of  $\mathcal{C} \setminus X, Y$ . To be specific, without loss of generality we assume that there is a non-uniform interspace  $\mathcal{C}[U,X]$ . If possible, we fix U such that  $\mathcal{C}[U,Y]$  is also non-uniform and also set W=U in this case; this is Case (a) in Figure 11. Otherwise, we fix a fiber W of  $\mathcal{C} \setminus X, Y$  such that  $\mathcal{C}[W,Y]$  is non-uniform if such a fiber exists. Then  $W \neq U$ ; this is Case (b) in Figure 11. If such a fiber does not exist, we again set W=U. In the last case,  $\mathcal{C}[W,Y]$  is uniform.

Since  $\mathcal{C}$  contains no interspace with a matching, Lemma 6.2 implies that  $\mathcal{C}[U,X] \simeq 2K_{2,2}$ . By the same reason we also have  $\mathcal{C}[W,Y] \simeq 2K_{2,2}$ , unless  $\mathcal{C}[W,Y]$  is uniform. If U=W and both  $\mathcal{C}[U,X]$  and  $\mathcal{C}[U,Y]$  are non-uniform, then Lemma 5.3 implies that these interspaces have skewed connection at U; see Figure 11(a).

Fix basis relations  $T \in \mathcal{C}[X,Y]$ ,  $T_X \in \mathcal{C}[U,X]$ , and  $T_Y \in \mathcal{C}[W,Y]$ . Enumerate the points in the fibers  $X = \{x_1, x_3, x_5, x_7\}$  and  $Y = \{y_2, y_4, y_6, y_8\}$  so that the indices correspond to the 8-cycle underlying T, as in Figure 11. By Part 3 of Lemma 5.2,

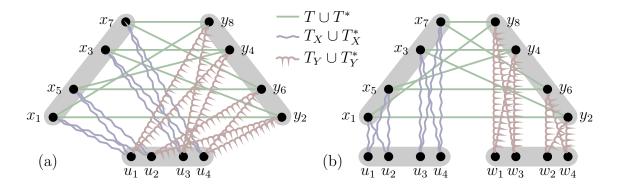


Figure 11: Proof of Lemma 6.1. Case (a): U = W. Case (b):  $U \neq W$ . In both cases, C[Y, W] is non-uniform.

the cell  $\mathcal{C}[X]$  contains a unique matching, namely

$$N_X = \{x_1 x_5, x_5 x_1, x_3 x_7, x_7 x_3\} \tag{31}$$

(corresponding to the two pairs of antipodal odd points on the 8-cycle). Therefore, Part 2 of the same lemma implies that C[U, X] determines exactly this matching in C[X]. We enumerate the points of  $U = \{u_1, u_2, u_3, u_4\}$  so that

$$T_X = \{u_1, u_2\} \times \{x_1, x_5\} \cup \{u_3, u_4\} \times \{x_3, x_7\}.$$

Note that C[X, U] determines the matching

$$M_X = \{u_1 u_2, u_2 u_1, u_3 u_4, u_4 u_3\}$$
(32)

in the cell C[U].

If U = W and both  $\mathcal{C}[U, X]$  and  $\mathcal{C}[U, Y]$  are non-uniform, then we suppose that

$$T_Y = \{u_1, u_3\} \times \{y_4, y_8\} \cup \{u_2, u_4\} \times \{y_2, y_6\},$$

as in Figure 11(a). Thus,  $T_Y$  determines the matching

$$M_Y = \{u_1u_3, u_3u_1, u_2u_4, u_4u_2\}$$

in C[W] = C[U]. This assumption causes no loss of generality because the coherent configuration  $C[X \cup Y \cup U]$  under the conditions  $C[X, Y] \simeq C_8$ ,  $C[X, U] \simeq 2K_{2,2}$ , and  $C[Y, U] \simeq 2K_{2,2}$  is unique up to combinatorial isomorphism. Indeed, the points of  $C[X \cup Y \cup U]$  can obviously be enumerated so that the fragments  $C[X \cup Y]$  and  $C[X \cup U]$  will look exactly as in Figure 11(a). Once this is fixed, the interspace C[U, Y] must determine the matching  $\{y_2y_6, y_6y_2, y_4y_8, y_8y_4\}$  in C[Y] corresponding to the two pairs of antipodal even points on the 8-cycle. By Lemma 5.3, the interspace C[Y, U] must determine a matching in C[U] different from  $M_X$ . One of these matchings, namely  $M_Y$ , appears in Figure 11(a), and the other of them results actually in the same picture by transposing the points  $u_1$  and  $u_2$ .

If  $U \neq W$ , then we enumerate  $W = \{w_1, w_2, w_3, w_4\}$  so that

$$T_Y = \{w_1, w_3\} \times \{y_4, y_8\} \cup \{w_2, w_4\} \times \{y_2, y_6\}.$$

In this case,

$$M_Y = \{w_1w_3, w_3w_1, w_2w_4, w_4w_2\},\$$

where  $M_Y$ , as above, denotes the matching determined by C[Y, W] in C[W]. For notational convenience, in the case that U = W we set  $w_i = u_i$  for each  $i \leq 4$ . Note that  $M_Y$  is well defined irrespectively of whether W = U or  $W \neq U$ .

 $(\Longrightarrow)$  Let  $f_0$  be an algebraic isomorphism from  $\mathcal{C} \setminus X, Y$  to a coherent configuration  $\mathcal{D}$ . Like in the proof of Lemma 5.1, it suffices to extend  $\mathcal{D}$  to a coherent configuration  $\mathcal{C}'$  and to extend  $f_0$  to an algebraic isomorphism f from  $\mathcal{C}$  to  $\mathcal{C}'$ .

For a fiber A of  $C \setminus X, Y$ , let  $A' = f_0(A)$  denote the fiber of  $\mathcal{D}$  corresponding to A under  $f_0$ . We fix an enumeration  $U' = \{u'_1, u'_2, u'_3, u'_4\}$  so that

$$f_0(M_X) = \{u_1'u_3', u_3'u_1', u_2'u_4', u_4'u_2'\}.$$
(33)

If W = U, then W' = U', and we set  $w'_i = u'_i$  for  $i \le 4$ . If  $W \ne U$ , then we fix an enumeration  $W' = \{w'_1, w'_2, w'_3, w'_4\}$  so that

$$f_0(M_Y) = \{w_1'w_3', w_3'w_1', w_2'w_4', w_4'w_2'\}.$$

We now construct  $\mathcal{C}'$  and f as follows. Let  $\phi_{UW}$  be the bijection from  $U \cup W$  onto  $U' \cup W'$  defined by  $\phi_{UW}(u_i) = u_i'$  and  $\phi_{UW}(w_i) = w_i'$ . Moreover, we take  $X' = \{x_1', x_3', x_5', x_7'\}$  and  $Y = \{y_2', y_4', y_6', y_8'\}$  such that  $X' \cap Y' = \emptyset$  and  $(X' \cup Y') \cap V(\mathcal{D}) = \emptyset$  and extend  $\phi_{UW}$  to a bijection from  $U \cup W \cup X \cup Y$  onto  $U' \cup W' \cup X' \cup Y'$  by setting  $\phi_{UW}(x_i) = x_i'$  and  $\phi_{UW}(y_i) = y_i'$ . The sets X' and Y' will be fibers of  $\mathcal{C}'$ . We build the fragments  $\mathcal{C}'[U' \cup X' \cup Y']$  and  $\mathcal{C}'[W' \cup X' \cup Y']$  as isomorphic copies of  $\mathcal{C}[U \cup X \cup Y]$  and  $\mathcal{C}[W \cup X \cup Y]$  under the map  $\phi_{UW}$ . Moreover, for any relation  $R \in \mathcal{C}[U \cup X \cup Y] \cup \mathcal{C}[W \cup X \cup Y]$  we set  $f(R) = \phi_{UW}(R)$ .

It remains, for each  $Z \in F(\mathcal{C})$  such that  $Z \notin \{X, Y, U, W\}$  to construct  $\mathcal{C}'[X', Z']$  and  $\mathcal{C}'[Y', Z']$  and to define f locally as a bijection from  $\mathcal{C}[X, Z]$  to  $\mathcal{C}'[X', Z']$  and  $\mathcal{C}[Y, Z]$  to  $\mathcal{C}'[Y', Z']$ . If  $\mathcal{C}[X, Z]$  is uniform, we set  $\mathcal{C}'[X', Z']$  also to be uniform, and correspondingly define  $f(X \times Z) = X' \times Z'$ . Similarly, if  $\mathcal{C}[Y, Z]$  is uniform, we set  $\mathcal{C}'[Y', Z']$  to be uniform and define  $f(Y \times Z) = Y' \times Z'$ .

Assume that  $\mathcal{C}[X,Z]$  is non-uniform. By Lemma 6.2,  $\mathcal{C}[X,Z] \simeq 2K_{2,2}$ . Recall that the cell  $\mathcal{C}[X]$  contains a unique matching basis relation, namely  $N_X$ . By Part 2 of Lemma 5.2,  $\mathcal{C}[Z,X]$  determines  $N_X$  in  $\mathcal{C}[X]$  and, hence, is directly connected to  $\mathcal{C}[U,X]$  at X. Lemma 5.3 implies that  $\mathcal{C}[Z,U] \simeq 2K_{2,2}$  and that the interspace  $\mathcal{C}[Z,U]$  has direct connections to  $\mathcal{C}[U,X]$  at U and to  $\mathcal{C}[X,Z]$  at Z. In particular,  $\mathcal{C}[Z,U]$  determines the same matching in  $\mathcal{C}[U]$  as  $\mathcal{C}[X,U]$ , namely  $M_X$ . Note that  $\mathcal{C}[Z,Y]$  must be uniform. If  $W \neq U$ , this follows by the choice of W and, if W = U, the non-uniformity of  $\mathcal{C}[Z,Y]$ , by the argument similar to the above, would imply that  $\mathcal{C}[Z,U]$  in  $\mathcal{C}[U]$  determines the matching  $M_Y$  rather than  $M_X$ .

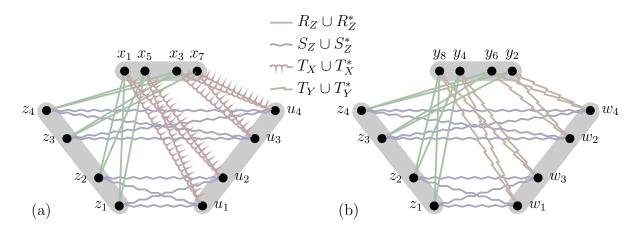


Figure 12: Proof of Lemma 6.1. (a)  $\mathcal{C}[X,Z]$  is non-uniform, and  $\mathcal{C}[Y,Z]$  is uniform: relations are named as in the proof; (b)  $\mathcal{C}[X,Z]$  is uniform, and  $\mathcal{C}[Y,Z]$  is non-uniform: now  $S_Z \in \mathcal{C}[Z,W]$  and  $R_Z \in \mathcal{C}[Y,Z]$ .

The rest of our argument is similar to the proof of Lemma 5.1. Fix a basis relation  $S_Z \in \mathcal{C}[Z, U]$ . Fix an enumeration  $Z = \{z_1, z_2, z_3, z_4\}$  such that

$$S_Z = \{z_1, z_2\} \times \{u_1, u_2\} \cup \{z_3, z_4\} \times \{u_3, u_4\}; \tag{34}$$

see Figure 12(a). Since  $f_0$  is an algebraic isomorphism from  $\mathcal{C} \setminus X, Y$  to  $\mathcal{D}$  and  $S_Z$  determines the matching  $M_X$  in  $\mathcal{C}[U]$ , the basis relation  $f_0(S_Z)$  determines the matching  $f_0(M_X)$  in  $\mathcal{D}[U']$ . Taking into account (33), the points of Z' can be enumerated so that

$$f_0(S_Z) = \{z_1', z_2'\} \times \{u_1', u_2'\} \cup \{z_3', z_4'\} \times \{u_3', u_4'\},\tag{35}$$

and we fix such an enumeration  $z'_1, z'_2, z'_3, z'_4$ . Note that  $\mathcal{C}[X, Z]$  consists of the basis relation

$$R_Z = \{x_1, x_5\} \times \{z_1, z_2\} \cup \{x_3, x_7\} \times \{z_3, z_4\}$$
(36)

and its complement  $X \times Z \setminus R_Z$ . We, therefore, define the interspace  $\mathcal{C}'[X', Z']$  as consisting of the relation

$$R'_{Z} = \{x'_{1}, x'_{5}\} \times \{z'_{1}, z'_{2}\} \cup \{x'_{3}, x'_{7}\} \times \{z'_{3}, z'_{4}\}$$
(37)

and its complement  $X' \times Z' \setminus R'_Z$ . This ensures that  $\mathcal{C}'[X' \cup U' \cup Z']$  is a coherent configuration combinatorially isomorphic to  $\mathcal{C}[X \cup U \cup Z]$ . Moreover, we define f on  $\mathcal{C}[X,Z]$  by setting

$$f(R_Z) = R_Z'. (38)$$

This ensures that f is an algebraic isomorphism from  $\mathcal{C}[X \cup U \cup Z]$  to  $\mathcal{C}'[X' \cup U' \cup Z']$ . Assume now that  $\mathcal{C}[Y, Z]$  is non-uniform. As was noticed, in this case the interspace  $\mathcal{C}[X, Z]$  must be uniform and, therefore, the fiber Z was not handled above. We construct  $\mathcal{C}'[Y', Z']$  and extend f to a map from  $\mathcal{C}[Y, Z]$  to  $\mathcal{C}'[Y', Z']$  similarly to the above, considering the interspaces  $C[Y, W] \simeq 2K_{2,2}$  and  $C[Z, W] \simeq 2K_{2,2}$ ; see Figure 12(b).

The construction of  $\mathcal{C}'$  and  $f: \mathcal{C} \to \mathcal{C}'$  is therewith complete. It remains to argue that  $\mathcal{C}'$  is indeed a coherent configuration and that f is indeed an algebraic isomorphism from  $\mathcal{C}$  to  $\mathcal{C}'$ . We use Lemma 3.4.

If A, B, C are fibers of  $C \setminus X, Y$ , then the assumptions of Lemma 3.4 are trivially true.

Let B=X and C=Y. If A=U or A=W, then the assumptions of Lemma 3.4 are ensured by the construction. Suppose that A=Z is a fiber of  $\mathcal{C}\setminus X,Y$  different from U and W. Recall that at least one of the interspaces  $\mathcal{C}[Z,X]$  and  $\mathcal{C}[Z,Y]$  is uniform. To be specific, assume that  $\mathcal{C}[Z,Y]$  is uniform; the other case is symmetric. Using the fact that any association scheme on 4 points is separable, we consider a bijection  $\phi_Z:Z\to Z'$  that is a combinatorial isomorphism from  $\mathcal{C}[Z]$  to  $\mathcal{D}[Z']$  inducing the restriction of  $f_0$  to  $\mathcal{C}[Z]$ . We stick to the enumeration  $z_1, z_2, z_3, z_4$  and  $z'_1, z'_2, z'_3, z'_4$  of points in Z and Z' fixed while constructing  $\mathcal{C}'[Z', X']$ . If  $\mathcal{C}[Z, X]$  is non-uniform, then either

$$\phi_Z(\{z_1, z_2\}) = \{z_1', z_2'\} \tag{39}$$

or  $\phi_Z(\{z_1, z_2\}) = \{z_3', z_4'\}$ . The association scheme  $\mathcal{C}[Z]$  has a combinatorial automorphism that maps each basis relation onto itself and swaps the sets  $\{z_1, z_2\}$  and  $\{z_3, z_4\}$ . Using this automorphism if needed, we can ensure Equality (39). Extend  $\phi_Z$  to a bijection  $\phi_Z: X \cup Y \cup Z \to X' \cup Y' \cup Z'$  by setting  $\phi(x_i) = x_i'$  and  $\phi(y_i) = y_i'$ . For the basis relations  $R_Z$  and  $R_Z'$  introduced by (36) and (37), from the definition of  $\phi_Z$  on  $X \cup Y$  and Equality (39) we derive that  $\phi_Z(R_Z) = R_Z'$ . Along with (38), this shows that  $\phi_Z$  is a combinatorial isomorphism from  $\mathcal{C}[X \cup Y \cup Z]$  to  $\mathcal{C}'[X' \cup Y' \cup Z']$  and that  $\phi_Z$  induces the restriction of f to  $\mathcal{C}[X \cup Y \cup Z]$ . Thus, the assumptions of Lemma 3.4 are fulfilled also in this case.

Assume now that C = X and A and B are fibers of  $C \setminus X, Y$ . If  $U \in \{A, B\}$ , then the assumptions of Lemma 3.4 are ensured by the construction. Suppose, therefore, that neither A nor B is equal to U. Our goal is to construct a bijection  $\phi_{AB}$  from  $X \cup A \cup B$  onto  $X' \cup A' \cup B'$  that is a combinatorial isomorphism from  $C[X \cup A \cup B]$  to  $C'[X' \cup A' \cup B']$  and that induces the restriction of f to  $C[X \cup A \cup B]$ . Like in the proof of Lemma 5.1, we split our analysis into three cases.

Case 1: Both C[A, X] and C[B, X] are uniform. The interspace C[A, B] can be uniform or of  $2K_{2,2}$ - or  $C_8$ -type. The structure of the subconfiguration  $C[A \cup B]$  in the last two cases is described by Parts 2 and 3 of Lemma 5.2. In each case, it is easy to see that the restriction of  $f_0$  to an algebraic isomorphism from  $C[A \cup B]$  to  $C'[A' \cup B']$  is induced by a combinatorial isomorphism  $\phi_0 : A \cup B \to A' \cup B'$ . We extend  $\phi_0$  to  $\phi_{AB}$  by setting  $\phi_{AB}(x_i) = x'_i$ .

Case 2: Exactly one of the interspaces C[A, X] and C[B, X], say C[A, X], is non-uniform. Like in the first case, C[A, B] can be uniform or of  $2K_{2,2}$ - or  $C_8$ -type. Again, let  $\phi_0: A \cup B \to A' \cup B'$  be a combinatorial isomorphism  $C[A \cup B]$  to  $C'[A' \cup B']$  inducing the restriction of  $f_0$  to  $C[A \cup B]$ . By Lemma 6.2,  $C[A, X] \simeq 2K_{2,2}$ , and we

consider the enumeration  $a_1, a_2, a_3, a_4$  of A and the enumeration  $a'_1, a'_2, a'_3, a'_4$  of A' that we have fixed for each such A; cf. (34) and (35). Let

$$M_A = \{a_1a_2, a_2a_1, a_3a_4, a_4a_3\}$$

and

$$M'_A = \{a'_1 a'_2, a'_2 a'_1, a'_3 a'_4, a'_4 a'_3\}$$

be the matchings determined by the interspaces C[U, A] in the cell C[A] and C'[U', A'] in C'[A']. By (34) and (35) applied to Z = A, we have  $f_0(M_A) = M'_A$ . It follows that either

$$\phi_0(\{a_1, a_2\}) = \{a'_1, a'_2\}$$
 and  $\phi_0(\{a_3, a_4\}) = \{a'_3, a'_4\}$ 

or

$$\phi_0(\{a_1, a_2\}) = \{a_3', a_4'\}$$
 and  $\phi_0(\{a_3, a_4\}) = \{a_1', a_2'\}.$ 

In the former case, we extend  $\phi_0$  to  $\phi_{AB}$  by  $\phi_{AB}(x_i) = x_i'$ . In the latter case, however, we have to swap the values of  $\phi_{AB}$  on X so that  $\phi_{AB}(\{x_1, x_5\}) = \{x_3', x_7'\}$  and  $\phi_{AB}(\{x_3, x_7\}) = \{x_1', x_5'\}$ . This ensures that  $\phi_{AB}(R_A) = R_A'$  for the basis relations  $R_A$  and  $R_A'$  as in (36) and (37). It follows from (38) that the restriction of f to  $\mathcal{C}[A \cup B \cup X]$  is induced by  $\phi_{AB}$ .

Case 3: Both C[A, X] and C[B, X] are non-uniform. Recall that, by Lemma 6.2, both  $C[A, X] \simeq 2K_{2,2}$  and  $C[B, X] \simeq 2K_{2,2}$ . Moreover, both C[A, X] and C[B, X] are directly connected to  $C[U, X] \simeq 2K_{2,2}$  at X. It follows by Lemma 5.3 that both  $C[A, U] \simeq 2K_{2,2}$  and  $C[B, U] \simeq 2K_{2,2}$  are directly connected to C[X, U] at U and, therefore, also to each other. Applying Lemma 5.3 once again, we conclude that  $C[A, B] \simeq 2K_{2,2}$  and the connections between C[A, B] with C[U, A] at C[U, B] at C[U, B] are direct. Using the enumeration of the fibers C[A, B] consists of the basis relation

$$Q_{AB} = \{a_1, a_2\} \times \{b_1, b_2\} \cup \{a_3, a_4\} \times \{b_3, b_4\}$$

and its complement  $A \times B \setminus Q_{AB}$ . Taking into account Equalities (34) and (35) for Z = A and Z = B, we conclude that

$$f_0(Q_{AB}) = \{a'_1, a'_2\} \times \{b'_1, b'_2\} \cup \{a'_3, a'_4\} \times \{b'_3, b'_4\}.$$

We know the structure of the coherent configuration  $C[A \cup B \cup U]$  up to the types of its cells C[A], C[B], and C[U]. In each case, the restriction of  $f_0$  to an algebraic isomorphism from  $C[A \cup B \cup U]$  to  $C'[A' \cup B' \cup U']$  is induced by a combinatorial isomorphism  $\phi_0 : A \cup B \cup U \to A' \cup B' \cup U'$ . Since  $\phi_0(Q_{AB}) = f_0(Q_{AB})$ , we have either

$$\phi_0(\{a_1, a_2\}) = \{a_1', a_2'\} \text{ and } \phi_0(\{b_1, b_2\}) = \{b_1', b_2'\}$$
(40)

or

$$\phi_0(\{a_1, a_2\}) = \{a_3', a_4'\}$$
 and  $\phi_0(\{b_1, b_2\}) = \{b_3', b_4'\}.$ 

Applying, if necessary, an appropriate combinatorial automorphism of  $C[A \cup B \cup U]$ , we can ensure Equality (40). We now extend  $\phi_0$  to  $\phi_{AB}$  by  $\phi_{AB}(x_i) = x_i'$ . Note that

$$\phi_{AB}(R_A) = R'_A$$
 and  $\phi_{AB}(R_B) = R'_B$ 

for the basis relations introduced by (36) and (37). Based on (38), we conclude that the restriction of f to  $\mathcal{C}[A \cup B \cup X]$  is induced by  $\phi_{AB}$ .

The analysis of fiber triples A, B, C such that C = X and  $A, B \in F(\mathcal{C} \setminus X, Y)$  is complete. The triple of fibers consisting of C = Y and  $A, B \in F(\mathcal{C} \setminus X, Y)$  are treated similarly.

 $(\longleftarrow)$  Let f be an algebraic isomorphism from  $\mathcal{C}$  to a coherent configuration  $\mathcal{C}'$ . For each fiber  $A \in F(\mathcal{C})$ , let A' = f(A) denote the corresponding fiber of  $\mathcal{C}'$ . Like in the proof of Lemma 5.1, denote the restriction of f to  $\mathcal{C} \setminus X, Y$  by  $f_0$  and note that  $f_0$  is an algebraic isomorphism from  $\mathcal{C} \setminus X, Y$  to the coherent configuration  $\mathcal{C}' \setminus X', Y'$ . Since  $\mathcal{C} \setminus X, Y$  is separable,  $f_0$  is induced by a combinatorial isomorphism  $\phi_0 : V(\mathcal{C}) \setminus (X \cup Y) \to V(\mathcal{C}') \setminus (X' \cup Y')$ . We have to extend  $\phi_0$  to a combinatorial isomorphism  $\phi : V(\mathcal{C}) \to V(\mathcal{C}')$  from  $\mathcal{C}$  to  $\mathcal{C}'$  that induces f.

We first solve a more modest task of defining  $\phi$  on  $X \cup Y$  so that  $\phi$  will be a combinatorial isomorphism from  $\mathcal{C}[X \cup Y \cup U \cup W]$  to  $\mathcal{C}'[X' \cup Y' \cup U' \cup W']$  inducing the restriction of f to an algebraic isomorphism between these subconfigurations. Let

$$u'_{i} = \phi_{0}(u_{i})$$
 and  $w'_{i} = \phi_{0}(w_{i})$  for  $i \leq 4$ .

Since f is an algebraic isomorphism,  $f(M_X)$  is a matching basis relation in  $\mathcal{C}'[U']$ ; see (32) and Figure 11. Since  $\phi_0$  induces the restriction of f to  $\mathcal{C}[U]$ ,

$$f(M_X) = \{u_1'u_2', u_2'u_1', u_3'u_4', u_4'u_3'\}.$$

Since f is an algebraic isomorphism,  $f(T_X)$  determines  $f(M_X)$  in  $\mathcal{C}'[U']$ . If  $\mathcal{C}[W,Y]$  is non-uniform, then we similarly have

$$f(M_Y) = \{w_1'w_3', w_3'w_1', w_2'w_4', w_4'w_2'\},\$$

and  $f(T_Y)$  determines  $f(M_Y)$  in  $\mathcal{C}'[W']$ , irrespectively of whether W = U or  $W \neq U$ . We enumerate  $X' = \{x'_1, x'_3, x'_5, x'_7\}$  and  $Y' = \{y'_2, y'_4, y'_6, y'_8\}$  so that

$$f(T_X) = \{u_1', u_2'\} \times \{x_1', x_5'\} \cup \{u_3', u_4'\} \times \{x_3', x_7'\}$$

$$\tag{41}$$

and

$$f(T_Y) = \{w_1', w_3'\} \times \{y_4', y_8'\} \cup \{w_2', w_4'\} \times \{y_2', y_6'\},\$$

the last equality under the assumption that C[W, Y] is non-uniform. Our first concern is to satisfy the constraints

$$\phi(\lbrace x_1, x_5 \rbrace) = \lbrace x_1', x_5' \rbrace \text{ and } \phi(\lbrace y_2, y_6 \rbrace) = \lbrace y_2', y_6' \rbrace. \tag{42}$$

This will ensure that

$$\phi(T_X) = f(T_X)$$
 and  $\phi(T_Y) = f(T_Y)$ ,

accomplishing our task locally on  $\mathcal{C}[X \cup U]$  and  $\mathcal{C}[Y \cup W]$ , the latter also if  $\mathcal{C}[W, Y]$  is uniform. We fulfill the first equality in (42) immediately just by setting

$$\phi(x_1) = x_1'$$
 and  $\phi(x_5) = x_5'$ .

It remains to ensure the second equality in (42) as well as the equality

$$\phi(T) = f(T) \tag{43}$$

for the 8-cycles  $T \in \mathcal{C}[X,Y]$  and  $f(T) \in \mathcal{C}'[X',Y']$ ; see Figure 11. Since f is an algebraic isomorphism, Equality (41) implies that

$$f(N_X) = \{x_1'x_5', x_5'x_1', x_3'x_7', x_7'x_3'\}$$

for the unique matching basis relation  $N_X \in \mathcal{C}[X]$  introduced by (31). Therefore  $x_1', x_5'$  and  $x_3', x_7'$  are the two pairs of diametrically opposite points on the 8-cycle f(T) that belong to X'. Similarly, if  $\mathcal{C}[W, Y]$  is non-uniform, then  $y_2', y_6'$  and  $y_4', y_8'$  are the two pairs of antipodal points on f(T) belonging to Y'. In fact, we can suppose this also if  $\mathcal{C}[W, Y]$  is uniform, as Y' can be enumerated arbitrarily in this case. Let y' be the common neighbor of  $x_1'$  and  $x_3'$  on f(T). We set

$$\phi(x_3) = x_3'$$
 and  $\phi(x_7) = x_7'$  if  $y' \in \{y_2', y_6'\}$ 

or

$$\phi(x_3) = x_7'$$
 and  $\phi(x_7) = x_3'$  if  $y' \in \{y_4', y_8'\}$ .

Assignment of the four values  $\phi(x_i)$  uniquely determines the four values  $\phi(y_i)$ . For example,  $\phi(y_1)$  is the point in Y' lying on f(T) between  $\phi(x_1)$  and  $\phi(x_3)$ . In each case, Conditions (42) and (43) are fulfilled.

Our modest task is fulfilled. Now, let  $Z \neq U, W$  be another fiber of  $\mathcal{C} \setminus X, Y$ . We have to verify that  $\phi$  is a combinatorial isomorphism from  $\mathcal{C}[X \cup Z]$  to  $\mathcal{C}'[X' \cup Z']$  and from  $\mathcal{C}[Y \cup Z]$  to  $\mathcal{C}'[Y' \cup Z']$  and that  $\phi$  induces f on these subconfigurations. We do it for  $\mathcal{C}[X \cup Z]$ ; the argument for  $\mathcal{C}[Y \cup Z]$  is similar.

If  $\mathcal{C}[X,Z]$  is uniform, we have nothing to do. Assume, therefore, that  $\mathcal{C}[X,Z]$  is non-uniform and, hence,  $\mathcal{C}[X,Z] \simeq 2K_{2,2}$ . Recall that the connection between  $\mathcal{C}[Z,X]$  and  $\mathcal{C}[U,X]$  at X must be direct; see Figure 12(a). Moreover,  $\mathcal{C}[Z,U] \simeq 2K_{2,2}$  is directly connected to  $\mathcal{C}[X,U]$  at U and to  $\mathcal{C}[X,Z]$  at Z. Let  $Z = \{z_1, z_2, z_3, z_4\}$  and, without loss of generality, suppose that  $\mathcal{C}[U,Z]$  and  $\mathcal{C}[X,Z]$  determine a matching  $\{z_1z_2, z_2z_1, z_3z_4, z_4z_3\}$  in  $\mathcal{C}[Z]$ . Thus,  $\mathcal{C}[Z,U]$  consists of the basis relation

$$S_Z = \{z_1, z_2\} \times \{u_1, u_2\} \cup \{z_3, z_4\} \times \{u_3, u_4\}$$

and its complement  $Z \times U \setminus S_Z$ , while  $\mathcal{C}[X,Z]$  consists of the basis relation

$$R_Z = \{x_1, x_5\} \times \{z_1, z_2\} \cup \{x_3, x_7\} \times \{z_3, z_4\}$$

and its complement  $X \times Z \setminus R_Z$ . Since  $f_0$  is induced by  $\phi_0$ , we have

$$f(S_Z) = \{z_1', z_2'\} \times \{u_1', u_2'\} \cup \{z_3', z_4'\} \times \{u_3', u_4'\}, \tag{44}$$

where  $z_i' = \phi_0(z_i)$ . Since f provides an algebraic isomorphism from  $\mathcal{C}[X \cup U \cup Z]$  to  $\mathcal{C}'[X' \cup U' \cup Z']$ , Equalities (44) and (41) imply that

$$f(R_Z) = \{x_1', x_5'\} \times \{z_1', z_2'\} \cup \{x_3', x_7'\} \times \{z_3', z_4'\},\$$

see Figure 12(a). Along with the first equality in (42), this shows that

$$f(R_Z) = \phi(R_Z).$$

We see that, as claimed,  $\phi$  is a combinatorial isomorphism from  $\mathcal{C}[X \cup Z]$  to  $\mathcal{C}'[X' \cup Z']$  inducing f.

The proof of Lemma 6.1 is complete.

# 7 Irredundant configurations: Preliminaries

Along with two other Cut-Down Lemmas (i.e., Lemmas 4.1 and 5.1), Lemma 6.1 reduces our task to deciding separability of a coherent configuration  $\mathcal{C}$  under the following three conditions:

- (1)  $\mathcal{C}$  is indecomposable;
- (2) all fibers of  $\mathcal{C}$  have size 4;
- (3) every non-uniform interspace of C is of type  $2K_{2,2}$ .

A coherent configuration satisfying Conditions (1)–(3) will be called *irredundant*.

## 7.1 Strict algebraic automorphisms

We begin with noticing that, for irredundant configurations, every algebraic isomorphism f gives rise to a combinatorial isomorphism  $\phi$ , even though  $\phi$  does not need to induce f on the whole coherent configuration.

**Lemma 7.1.** Suppose that a coherent configuration C is irredundant. If f is an algebraic isomorphism from C to a coherent configuration C', then there exists a combinatorial isomorphism  $\phi$  from C to C' such that  $\phi$  induces f on the cell C[X] for each fiber  $X \in F(C)$ .

Proof. For a fiber  $X \in F(\mathcal{C})$ , let X' = f(X) denote the corresponding fiber of  $\mathcal{C}'$ . We construct  $\phi$  locally as a bijection  $\phi: X \to X'$  for each  $X \in F(\mathcal{C})$ . The restriction of f to  $\mathcal{C}[X]$  is an algebraic isomorphism from the cell  $\mathcal{C}[X]$  to the cell  $\mathcal{C}'[X']$ . It is easy to check that all 4-point association schemes are separable. Using this fact, we set  $\phi: X \to X'$  to be a combinatorial isomorphism from  $\mathcal{C}[X]$  to  $\mathcal{C}'[X']$  inducing f on  $\mathcal{C}[X]$ . It remains to show that  $\phi$  defined in this way is also a partition isomorphism from  $\mathcal{C}[X,Y]$  to  $\mathcal{C}'[X',Y']$  for any two fibers  $X,Y \in F(\mathcal{C})$ .

Assume first that the interspace C[X,Y] is uniform. Since an algebraic isomorphism preserves the valency of a basis relation (see [10, Corollary 2.3.20]), the

interspace  $\mathcal{C}'[X',Y']$  is also uniform. Thus,  $\mathcal{C}[X,Y]$  consists of the single basis relation  $X \times Y$ , and  $\mathcal{C}'[X',Y']$  consists of the single basis relation  $X' \times Y'$ . We are done just because  $\phi(X \times Y) = X' \times Y'$ , as trivially follows from the equalities  $\phi(X) = X'$  and  $\phi(Y) = Y'$ .

Assume now that the interspace C[X,Y] is non-uniform, that is,  $C[X,Y] \simeq 2K_{2,2}$ . Since f preserves the valency of each basis relation in C[X,Y], we must have either  $C'[X',Y'] \simeq 2K_{2,2}$  or  $C'[X',Y'] \simeq C_8$ . The latter possibility is actually excluded. Indeed, let R be a basis relation in C[X,Y]. For the matching basis relation M determined by R in the cell C[X] according to Part 2 of Lemma 5.2, we have  $p_{RR^*}^M = 2$ . If  $C'[X',Y'] \simeq C_8$ , then Part 3 of Lemma 5.2 implies that the cell C'[X'] contains a single matching basis relation M'. For this matching we, however, have  $p_{f(R)f(R)^*}^{M'} = 0$  and, therefore,  $M' \neq f(M)$ .

Thus,  $\mathcal{C}'[X',Y'] \simeq 2K_{2,2}$ . Specifically, suppose that  $\mathcal{C}[X,Y]$  consists of the basis relation

$$R = \{x_1, x_2\} \times \{y_1, y_2\} \cup \{x_3, x_4\} \times \{y_3, y_4\}$$

and its complement  $X \times Y \setminus R$ , and  $\mathcal{C}'[X',Y']$  consists of the basis relation

$$f(R) = \{x_1', x_2'\} \times \{y_1', y_2'\} \cup \{x_3', x_4'\} \times \{y_3', y_4'\}$$

and its complement  $X' \times Y' \setminus f(R)$ . By Part 2 of Lemma 5.2,  $\mathcal{C}[X,Y]$  determines the matching basis relations

$$M = \{x_1x_2, x_2x_1, x_3x_4, x_4x_3\}$$

in the cell  $\mathcal{C}[X]$  and

$$N = \{y_1y_2, y_2y_1, y_3y_4, y_4y_3\}$$

in the cell C[Y], while C'[X', Y'] determines

$$M' = \{x_1'x_2', x_2'x_1', x_3'x_4', x_4'x_3'\}$$

in C'[X'] and

$$N' = \{y_1'y_2', y_2'y_1', y_3'y_4', y_4'y_3'\}$$

in  $\mathcal{C}'[Y']$ . Since f is an algebraic isomorphism, we have f(M) = M' and f(N) = N'. Since  $\phi$  induces f both on  $\mathcal{C}[X]$  and  $\mathcal{C}[Y]$ , this implies that  $\phi(M) = M'$  and  $\phi(N) = N'$ . Therefore, either  $\phi(\{x_1, x_2\}) = \{x_1, x_2\}$  or  $\phi(\{x_1, x_2\}) = \{x_3, x_4\}$ , and either  $\phi(\{y_1, y_2\}) = \{y_1, y_2\}$  or  $\phi(\{y_1, y_2\}) = \{y_3, y_4\}$ . There are four cases altogether. In two of them we have  $\phi(R) = f(R)$ , while  $\phi(R) = X' \times Y' \setminus f(R)$  in the other two cases. In each case,  $\phi$  is a partition isomorphism from  $\mathcal{C}[X, Y]$  to  $\mathcal{C}'[X', Y']$ . We conclude that  $\phi$  is a combinatorial isomorphism from  $\mathcal{C}$  to  $\mathcal{C}'$ .

Lemma 7.1 implies that, if a coherent configuration  $\mathcal{C}$  is irredundant, then  $\mathcal{C} \cong_{alg} \mathcal{C}'$  implies  $\mathcal{C} \cong_{comb} \mathcal{C}'$ . This has the following practical consequence: An irredundant configuration  $\mathcal{C}$  is separable if and only if every algebraic *automorphism* of  $\mathcal{C}$  is induced by a combinatorial automorphism of  $\mathcal{C}$ . Moreover, we call an algebraic automorphism f of  $\mathcal{C}$  strict if f is the identity on each cell  $\mathcal{C}[X]$  for  $X \in \mathcal{F}(\mathcal{C})$ .

**Lemma 7.2.** An irredundant coherent configuration C is separable if and only if every strict algebraic automorphism of C is induced by a combinatorial automorphism of C.

Proof. The direction 'only if' follows directly from the definition of a separable coherent configuration. For the other direction, assume that every strict algebraic automorphism of  $\mathcal{C}$  is induced by a combinatorial automorphism. We have to prove that  $\mathcal{C}$  is separable. Let f be an algebraic isomorphism from  $\mathcal{C}$  to  $\mathcal{C}'$ . Let  $\phi$  be a combinatorial isomorphism  $\phi:V(\mathcal{C})\to V(\mathcal{C}')$  from  $\mathcal{C}$  to  $\mathcal{C}'$  as in Lemma 7.1. Consider the composition  $g=\phi^{-1}\circ f$ , where  $\phi^{-1}$  is understood as the induced map from  $\mathcal{C}'$  to  $\mathcal{C}$ . Since  $\phi^{-1}$  is an algebraic automorphism from  $\mathcal{C}'$  to  $\mathcal{C}$ , the composition g is an algebraic automorphism of  $\mathcal{C}$ . Since  $\phi$  induces f on each cell of  $\mathcal{C}$ , this algebraic automorphism is strict. Note that  $f=\phi\circ g$ , where  $\phi$  is understood as the induced map from  $\mathcal{C}$  to  $\mathcal{C}'$ . By the assumption, g is induced by a combinatorial automorphism  $\psi$  of  $\mathcal{C}$ . It follows that f is induced by the combinatorial isomorphism  $\phi\circ\psi$  from  $\mathcal{C}$  to  $\mathcal{C}'$ .

Denote the set of strict algebraic automorphisms of a coherent configuration  $\mathcal{C}$  by  $\mathbb{A}(\mathcal{C})$ . Note that  $\mathbb{A}(\mathcal{C})$  is a group of permutations of the set  $\mathcal{C}$ . Furthermore, let  $\mathbb{A}^*(\mathcal{C})$  denote the set of those strict algebraic automorphisms of  $\mathcal{C}$  which are induced by combinatorial automorphisms of  $\mathcal{C}$ .

**Lemma 7.3.**  $\mathbb{A}^*(\mathcal{C})$  is a subgroup of  $\mathbb{A}(\mathcal{C})$ .

*Proof.* If f and h are in  $\mathbb{A}^*(\mathcal{C})$ , then they are induced by combinatorial automorphisms  $\phi$  and  $\psi$  respectively. Note that the product fh is induced by the combinatorial isomorphism  $\phi\psi$  and, therefore, fh is in  $\mathbb{A}^*(\mathcal{C})$  as well.

Similarly, we call a combinatorial automorphism  $\phi$  of  $\mathcal{C}$  strict if  $\phi$  takes every basis relation in each cell  $\mathcal{C}[X]$  onto itself. Obviously, a strict combinatorial automorphism induces a strict algebraic automorphism. Moreover, if a combinatorial automorphism  $\phi$  induces a strict algebraic automorphism, then  $\phi$  must be strict itself. We denote the set of strict combinatorial automorphisms of a coherent configuration  $\mathcal{C}$  by  $\mathbb{C}(\mathcal{C})$ . Note that  $\mathbb{C}(\mathcal{C})$  is a group of permutations on the point set  $V(\mathcal{C})$ . Furthermore, we call a combinatorial automorphism  $\phi$  of  $\mathcal{C}$  color-preserving if  $R^{\phi} = R$  for every basis relation  $R \in \mathcal{C}$ . The term is justified by the fact that  $\phi$  is a color-preserving automorphism of  $\mathcal{C}$  if any only if  $\phi$  is an automorphism of an (arbitrarily chosen) colored version  $\tilde{\mathcal{C}}$  of  $\mathcal{C}$ . Note that  $\phi$  is color-preserving if it induces the identity  $\mathrm{id}_{\mathcal{C}}$ . Obviously, a color-preserving combinatorial automorphism is strict, and the set  $\mathbb{C}_0(\mathcal{C})$  of all color-preserving automorphisms is a subgroup of  $\mathbb{C}(\mathcal{C})$ .

**Lemma 7.4.**  $\mathbb{C}(\mathcal{C})/\mathbb{C}_0(\mathcal{C}) \cong \mathbb{A}^*(\mathcal{C})$ , where  $\cong$  denotes isomorphism of groups.

*Proof.* Suppose that a permutation  $\phi$  of the point set  $V(\mathcal{C})$  is a strict combinatorial automorphism of  $\mathcal{C}$ . In this case, let  $\bar{\phi}$  denote the induced permutation of  $\mathcal{C}$ . The map  $\phi \mapsto \bar{\phi}$  is a homomorphism from the group  $\mathbb{C}(\mathcal{C})$  onto the group  $\mathbb{A}^*(\mathcal{C})$  whose kernel is  $\mathbb{C}_0(\mathcal{C})$ . The lemma immediately follows from the first isomorphism theorem.

**Lemma 7.5.** If C is irredundant, then  $\mathbb{C}(C) \cong \prod_{X \in F(C)} \mathbb{C}_0(C[X])$ .

*Proof.* To prove that  $\mathbb{C}(\mathcal{C})$  is isomorphic to a subgroup of  $\prod_{X \in F(\mathcal{C})} \mathbb{C}_0(\mathcal{C}[X])$ , consider an arbitrary  $\phi$  in  $\mathbb{C}(\mathcal{C})$ . Since each fiber X is invariant under  $\phi$ , this permutation is split into the product  $\phi = \prod_{X \in F(\mathcal{C})} \phi_X$ , where  $\phi_X$  is the identity outside X. By the definition of a strict automorphism, the restriction of  $\phi_X$  to X belongs to  $\mathbb{C}_0(\mathcal{C}[X])$ .

Let us prove that  $\prod_{X \in F(\mathcal{C})} \mathbb{C}_0(\mathcal{C}[X])$  is isomorphic to a subgroup of  $\mathbb{C}(\mathcal{C})$ . Consider  $\phi = \prod_{X \in F(\mathcal{C})} \phi_X$ , where  $\phi_X \in \mathbb{C}_0(\mathcal{C}[X])$  is defined outside X by identity. To show that  $\phi \in \mathbb{C}(\mathcal{C})$ , it is enough to prove that each  $\phi_X$  is a strict combinatorial automorphism of  $\mathcal{C}$ . This reduces to proving that, for any fiber  $Y \neq X$ , the partition  $\mathcal{C}[X,Y]$  is invariant under  $\phi_X$ . This is clear if  $\mathcal{C}[X,Y]$  is uniform. If the interspace  $\mathcal{C}[X,Y]$  is non-uniform, that is, consists of two basis relations  $R_1$  and  $R_2$ , then  $\mathcal{C}[X,Y]$  determines a matching basis relation M in the cell  $\mathcal{C}[X]$ . Since  $\phi_X(M) = M$  and  $\phi_X$  is the identity on Y, we see that  $\phi_X$  either fixes each of  $R_1$  and  $R_2$  or transposes them.

If a coherent configuration  $\mathcal{C}$  is irredundant, then every cell  $\mathcal{C}[X]$  is either of  $F_4$ -, or  $C_4$ -, or  $C_4$ -type; see Figure 1. In each of these cases, the group  $\mathbb{C}_0(\mathcal{C}[X])$  is clear. In particular, if  $\mathcal{C}[X]$  is of  $F_4$ -type, i.e., the factorization of X into three matchings, then  $\mathbb{C}_0(\mathcal{C}[X])$  is isomorphic to the Klein four-group. Specifically, this is the group K(X) of all such permutations  $\phi: X \to X$  that, for every two points  $x, x' \in X$ , either  $\phi(\{x, x'\}) = \{x, x'\}$  or  $\phi(\{x, x'\}) = X \setminus \{x, x'\}$ . If  $X = \{x_1, x_2, x_3, x_4\}$ , then

$$K(X) = {id_X, (x_1x_2)(x_3x_4), (x_1x_3)(x_2x_4), (x_1x_4)(x_2x_3)}.$$

Denote the three matching relations on X by M, N, and L, say,

$$M = \{x_1x_2, x_2x_1, x_3x_4, x_4x_3\},\$$

$$N = \{x_1x_3, x_3x_1, x_2x_4, x_4x_2\},\$$

$$L = \{x_1x_4, x_4x_1, x_2x_3, x_3x_2\}.$$

We will use the depicted colors for these relations in relevant figures. Any permutation  $\phi$  in K(X) preserves each of the matchings, that is,  $\phi(M) = M$ ,  $\phi(N) = N$ ,  $\phi(L) = L$ . If  $\phi$  preserves a matching, then two cases are possible: the matched pairs are either preserved or swapped. We say that  $\phi$  fixes the matching in the former case and that  $\phi$  flips the matching in the latter case. For example,  $\phi = (x_1x_2)(x_3x_4)$  fixes M and flips each of N and L. To emphasize on this, we will use also the notation  $\phi_{NL} = \phi_{LN} = (x_1x_2)(x_3x_4)$ . In this notation,

$$K(X) = \{ \mathrm{id}_X, \phi_{NL}, \phi_{ML}, \phi_{MN} \}, \tag{45}$$

where  $\phi_{ML} = (x_1x_3)(x_2x_4)$  fixes N and flips both M and L, and similarly for  $\phi_{MN}$ . Thus, Lemma 7.5 gives us a complete explicit description of the group  $\mathbb{C}(\mathcal{C})$ . A representation of the subgroup  $\mathbb{C}_0(\mathcal{C})$  by a set of generators is efficiently computable as explained in [1] as this is the automorphism group of a graph of color multiplicity 4 underlying any colored version  $\tilde{\mathcal{C}}$  of  $\mathcal{C}$ ; see Section 10. By Lemma 7.4, this makes the group  $\mathbb{A}^*(\mathcal{C})$  fully comprehensible. Since  $\mathcal{C}$  is separable exactly when  $\mathbb{A}(\mathcal{C}) = \mathbb{A}^*(\mathcal{C})$ , we can decide separability if we can efficiently find an explicit description of the group  $\mathbb{A}(\mathcal{C})$ . From now on, we focus on this task.

Call a permutation f on  $\mathcal{C}$  bound if f is the identity on each cell, maps each interspace onto itself, and satisfies the condition  $f(R^*) = f(R)^*$  for every basis relation R of  $\mathcal{C}$ . Since the last condition is obeyed by any algebraic isomorphism, every strict algebraic automorphism is bound. If  $\mathcal{C}[X,Y] \simeq 2K_{2,2}$ , then for a bound permutation f there are two possibilities. Specifically, suppose that  $\mathcal{C}[X,Y]$  partitions  $X \times Y$  into two parts  $R_1$  and  $R_2$ . We say that f fixes  $\mathcal{C}[X,Y]$  if

$$f(R_i) = R_i$$

and that f switches C[X,Y] if

$$f(R_i) = R_{3-i}$$

for i = 1, 2. Note that, if f switches  $\mathcal{C}[X, Y]$ , then it switches also  $\mathcal{C}[Y, X]$ . Given a set S of pairs  $\{X, Y\}$  such that  $\mathcal{C}[X, Y]$  is non-uniform, let  $f_S$  denote the bijection from  $\mathcal{C}$  onto itself which switches the interspace  $\mathcal{C}[X, Y]$  as well as the interspace  $\mathcal{C}[Y, X]$  for each  $\{X, Y\} \in S$  and leaves the rest of  $\mathcal{C}$  fixed. Thus, every bound permutation of  $\mathcal{C}$  coincides with  $f_S$  for some S. Conversely, every  $f_S$  is a bound permutation, but not all  $f_S$  must be algebraic automorphisms.

Thus, we have to describe the class of those S for which  $f_S$  is an algebraic automorphism. We begin our analysis with two instructive special cases in Subsections 8 and 9, and then consider the general case in Subsection 10. Prior to this we do some preliminary work in Subsection 7.2.

#### 7.2 The case of three fibers

Let f be a bound permutation of  $\mathcal{C}$ . Lemma 3.4 reduces verification of whether or not f is a strict algebraic automorphism of  $\mathcal{C}$  to local verification of this on all 3-fiber subconfigurations  $\mathcal{C}[X \cup Y \cup Z]$ . Thus, the case of coherent configurations with three fibers is quite important and we consider it here.

We call an irredundant configuration C skew-connected if C contains no directly connected interspaces.

**Lemma 7.6.** Let C be an irredundant coherent configuration with  $F(C) = \{X, Y, Z\}$  and f be a bound permutation of the set of basis relations of C.

- 1. If C is skew-connected, then f is an algebraic automorphism of C.
- 2. Suppose that C is not skew-connected. Then f is an algebraic automorphism of C if and only if either  $f = id_C$  or f makes exactly two switches of interspaces (switching an interspace and its transpose is counted as a single switch).

Proof. 1. It suffices to show that f is induced by some combinatorial automorphism  $\phi$  of  $\mathcal{C}$ . Let  $f_{XY}$  denote the restriction of f to  $\mathcal{C}[X,Y] \cup \mathcal{C}[Y,X]$  and extend it to the whole  $\mathcal{C}$  by identity. Define  $f_{YZ}$  and  $f_{XZ}$  similarly. Since  $f = f_{XY} \circ f_{YZ} \circ f_{XZ}$ , it is enough to check that each of the three permutations of  $\mathcal{C}$  are induced by a combinatorial automorphism of  $\mathcal{C}$ . We show this for  $f_{XY}$ , and the same argument applies as well for the other two cases. If  $\mathcal{C}[X,Y]$  is uniform or if f fixes  $\mathcal{C}[X,Y]$ , then  $f = \mathrm{id}_{\mathcal{C}}$  is induced by  $\mathrm{id}_{X \cup Y \cup Z}$ . Suppose that f switches  $\mathcal{C}[X,Y]$ . Let M be the matching basis relation of  $\mathcal{C}[X]$  determined by the interspace  $\mathcal{C}[Y,X]$  according to Lemma 5.2. If the interspace  $\mathcal{C}[Z,X]$  is non-uniform, it determines another matching relation L in L i

2. Since  $\mathcal{C}$  is not skew-connected, it contains two non-uniform directly connected interspaces and, therefore, Lemma 5.3 implies that all interspaces of  $\mathcal{C}$  are non-uniform and all connections between them are direct. Recall that f is an algebraic automorphism if and only if  $p_{ST}^R = p_{f(S)f(T)}^{f(R)}$  for all triples of basis relations  $R, S, T \in \mathcal{C}$ . This equality holds for every bound f if all three relations R, S, T are either in  $\mathcal{C}[X \cup Y]$ , or in  $\mathcal{C}[X \cup Z]$ , or in  $\mathcal{C}[Y \cup Z]$ ; cf. the proof of Part 1. The only situation that requires some care is when every interspace of  $\mathcal{C}$  contains one of the relations R, S, and T or their transposes. In any case of this kind, we have either  $p_{ST}^R = 2$  or  $p_{ST}^R = 0$ . The lemma follows from the observation that the value of  $p_{ST}^R$  switches from 2 to 0 or vice versa whenever we complement one of the relations. Specifically, let  $R^c = X \times Y \setminus R$  for a basis relation  $R \in \mathcal{C}[X,Y]$ . Using this notation also for other interspaces, we have

$$p_{ST}^R \neq p_{ST}^{R^c} = p_{S^cT}^R = p_{ST^c}^R \tag{46}$$

for any triple R, S, T under consideration. The inequality in (46) implies that any f making exactly one switch is not an algebraic automorphism. Applying (46) twice, we see that f making two switches is an algebraic automorphism. Applying (46) once again, we see that f making three switches is not an algebraic automorphism.  $\square$ 

# 8 Irredundant configurations: The CFI case

Let  $\mathcal{C}$  be an irredundant configuration. Like in the case of reduced Klein configurations [14], we define the *fiber graph* of  $\mathcal{C}$ , denoted by  $F_{\mathcal{C}}$ , as follows:

- The vertices of  $F_{\mathcal{C}}$  are the fibers of  $\mathcal{C}$ , i.e.,  $V(F_{\mathcal{C}}) = F(\mathcal{C})$ ;
- Two fibers X and Y are adjacent in  $F_{\mathcal{C}}$  if the interspace  $\mathcal{C}[X,Y]$  is non-uniform.

Recall that irredundant configurations are indecomposable. This implies that  $F_{\mathcal{C}}$  is connected.

As usually,  $\Delta(G)$  (resp.,  $\delta(G)$ ) denotes the maximum (resp., minimum) degree of a vertex in the graph G.

We now consider coherent configurations corresponding to the classical CFI construction [9] of graphs of color multiplicity 4 not amenable to k-WL. Recall that an irredundant configuration  $\mathcal{C}$  is skew-connected if  $\mathcal{C}$  contains no directly connected interspaces. Note that  $\Delta(F_{\mathcal{C}}) \leq 3$  in this case. Part 3 of the following lemma is reminiscent of [9, Lemma 6.2].

**Lemma 8.1.** If C is skew-connected, then the following is true.

- **1.**  $\mathbb{A}(C) = \{ f_S : S \subseteq E(F_C) \}.$
- **2.** If  $\delta(F_{\mathcal{C}}) \leq 2$ , then every  $f_S$  is induced by a combinatorial automorphism of  $\mathcal{C}$ .
- **3.** If  $\delta(F_C) = 3$ , i.e.,  $F_C$  is a regular graph of degree 3, then  $f_S$  is induced by a combinatorial automorphism of C exactly when |S| is even.

*Proof.* 1. This part follows directly from Lemma 3.4 and Part 1 of Lemma 7.6.

2. Note that  $f_S \circ f_{S'} = f_{S \triangle S'}$ , where  $\circ$  denotes the group operation in  $\mathbb{A}(\mathcal{C})$ , i.e., the composition of permutations. This implies that the set  $\mathbb{A}(\mathcal{C}) = \{f_S\}_S$  is a commutative group with every element having order 2. For  $s \in E(F_{\mathcal{C}})$ , denote  $f_s = f_{\{s\}}$ . The group  $\mathbb{A}(\mathcal{C})$  is generated by the set  $\{f_s : s \in E(F_{\mathcal{C}})\}$ . Indeed, if  $S = \{s_1, \ldots, s_k\}$ , then obviously  $f_S = f_{s_1} \circ \ldots \circ f_{s_k}$ . Therefore, it suffices to prove that, if  $\delta(F_{\mathcal{C}}) \leq 2$ , then each  $f_s$  is induced by a combinatorial automorphism of  $\mathcal{C}$ .

Let  $s = \{X, Y\}$ . Suppose first that the degree of X in  $F_{\mathcal{C}}$  is 2. This means that X is incident to two non-uniform interspaces of  $\mathcal{C}$ . One of them is  $\mathcal{C}[X, Y]$ , and let  $\mathcal{C}[X, Z]$  be the other one. By Part 2 of Lemma 5.2, each of the interspaces  $\mathcal{C}[Y, X]$  and  $\mathcal{C}[Z, X]$  determines a matching in the cell  $\mathcal{C}[X]$ . Denote these matchings by M and L respectively and note that  $M \neq L$  because  $\mathcal{C}$  is skew-connected. Therefore,  $\mathcal{C}[X] \simeq F_4$ . Let N be the third matching in  $\mathcal{C}[X]$ . Consider the permutation  $\phi_{MN}$  as in (45) and extend it to a permutation of the entire point set  $V = V(\mathcal{C})$  by identity outside X. Since N is not determined by any incident interspace,  $f_s$  is induced by  $\phi_{MN}$ .

Suppose now that X has degree 1 in  $F_{\mathcal{C}}$ . As above, let M be the matching determined in  $\mathcal{C}[X]$  by the interspace  $\mathcal{C}[Y,X]$ . Furthermore, let N be another matching relation on X. If  $\mathcal{C}[X] \simeq F_4$  or  $\mathcal{C}[X] \simeq C_4$ , then  $f_s$  is induced by  $\phi_{MN}$  by the same reason as above. If  $\mathcal{C}[X] \simeq \vec{C}_4$ , then this does not work because  $\phi_{MN}$  is not a strict combinatorial automorphism of  $\mathcal{C}[X]$ . In this case, let  $x_1, x_2, x_3, x_4$  be an enumeration of X along a non-matching basis relation of  $\mathcal{C}[X]$  (which is a directed 4-cycle). Then  $f_s$  is induced by the cyclic permutation  $(x_1x_2x_3x_4)$  because, as easily seen, this permutation flips M.

The case that both X and Y have degree 3 in  $F_{\mathcal{C}}$  can be reduced to the case above. Indeed, suppose that  $s_1 = \{A, B\}$  and  $s_2 = \{A, C\}$  are two adjacent edges in  $F_{\mathcal{C}}$ . Let M be the matching in the cell  $\mathcal{C}[A]$  determined by the interspace  $\mathcal{C}[B, A]$  and N be the matching in  $\mathcal{C}[A]$  determined by  $\mathcal{C}[C, A]$ . Note that

$$f_{s_1} \circ f_{s_2} = \phi_{MN}, \tag{47}$$

where  $\phi_{MN}$  is the permutation of  $\mathcal{C}$  induced by the permutation of V that flips each of M and N and is the identity outside A. Since all permutations under consideration are involutive, we infer from (47) that

$$f_{s_1} = \phi_{MN} \circ f_{s_2}.$$

It immediately follows that  $f_{s_1}$  is induced by a combinatorial automorphism if and only if  $f_{s_2}$  is induced by a combinatorial automorphism. By the connectedness of  $F_{\mathcal{C}}$ , this implies that all  $f_s$  are induced by combinatorial automorphisms if this is true for at least one of them, which is the case as we already know.

3. We first prove by induction on n that, if |S| = 2n, then  $f_S$  is induced by a combinatorial automorphism. If n = 0, then  $f_{\emptyset} = \mathrm{id}_{\mathcal{C}}$ , and the claim is trivially true.

Consider next the case that n=1, i.e.,  $S=\{s_1,s_2\}$ . If  $s_1$  and  $s_2$  are adjacent in  $F_{\mathcal{C}}$ , then  $f_S=f_{s_1}\circ f_{s_2}$  is induced by a combinatorial automorphism  $\phi_{MN}$  as in (47). Otherwise, consider a sequence  $s_1,r_1,\ldots,r_k,s_2$  of successive edges along a path in  $F_{\mathcal{C}}$ . Such a path exists because  $F_{\mathcal{C}}$  is connected. Note that

$$f_S = f_{s_1} \circ f_{s_2} = f_{s_1} \circ (f_{r_1} \circ f_{r_1}) \circ \dots \circ (f_{r_k} \circ f_{r_k}) \circ f_{s_2}$$
  
=  $(f_{s_1} \circ f_{r_1}) \circ (f_{r_1} \circ f_{r_2}) \circ \dots \circ (f_{r_{k-1}} \circ f_{r_k}) \circ (f_{r_k} \circ f_{s_2}).$ 

Since each of the factors  $f_{s_1} \circ f_{r_1}$ ,  $f_{r_i} \circ f_{r_{i+1}}$ , and  $f_{r_k} \circ f_{s_2}$  is induced by a combinatorial automorphism, this is true also for  $f_S$ .

Suppose now that n > 1. Let  $s_1$  and  $s_2$  be two elements of S. We have

$$f_S = f_{\{s_1, s_2\}} \circ f_{S \setminus \{s_1, s_2\}}.$$

By the induction assumption, both factors are induced by a combinatorial automorphism, so this must be true as well for  $f_S$ .

For the other direction, assume that |S| is odd. Let  $s \in S$ . We have

$$f_S = f_s \circ f_{S \setminus \{s\}}.$$

We already know that the second factor is induced by a combinatorial automorphism. This implies that  $f_S$  is induced by a combinatorial automorphism if and only if this is so for  $f_s$ . Therefore, it suffices<sup>3</sup> to prove that  $f_s$  is not induced by a combinatorial automorphism for any s.

Assume to the contrary that  $f_s$  is induced by a combinatorial automorphism  $\phi$ . Note that  $\phi$  must be strict and, by Lemma 7.5,

$$\phi = \prod_{X \in F(\mathcal{C})} \phi_X,\tag{48}$$

where  $\phi_X \in K(X)$  is defined outside X by identity. Consider a factor  $\phi_X$  that is non-identity; at least one such factor must exist. Suppose that  $\phi_X = \phi_{MN}$  for

<sup>&</sup>lt;sup>3</sup>As an alternative argument, note that, if we show that at least one  $f_s$  does not belong to  $\mathbb{A}^*(\mathcal{C})$ , then this will imply that  $\mathbb{A}^*(\mathcal{C})$  is a subgroup of  $\mathbb{A}(\mathcal{C})$  of index 2.

matchings M and N in  $\mathcal{C}[X]$ . Since X has degree 3 in  $F_{\mathcal{C}}$ , the matching M must be determined by an interspace  $\mathcal{C}[Y,X]$ , and N must be determined by an interspace  $\mathcal{C}[Z,X]$ . Let  $s_1 = \{X,Y\}$  and  $s_2 = \{X,Z\}$ . Accordingly with (47), we now have

$$\phi_X = f_{s_1} \circ f_{s_2},$$

where  $\phi_X$  is understood as the induced permutation of  $\mathcal{C}$ . Along with (48), this implies that

$$f_s = f_{s_1} \circ \ldots \circ f_{s_{2k}}$$

or, equivalently,

$$f_s \circ f_{s_1} \circ \ldots \circ f_{s_{2k}} = \mathrm{id}_{\mathcal{C}}.$$

After all possible cancellations of pairs of equal factors, the product in the left hand side is non-empty and consists of pairwise distinct factors, which yields a contradiction.

Corollary 8.2. A skew-connected coherent configuration C is separable if and only if  $\delta(F_C) \leq 2$ .

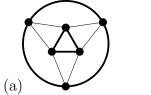
Remark 8.3. Let  $\mathcal{C}$  be a skew-connected coherent configuration with  $\delta(F_{\mathcal{C}}) = 3$ . Denote the number of fibers in  $\mathcal{C}$  by n. Then the fiber graph  $F_{\mathcal{C}}$  has n vertices and  $m = \frac{3}{2}n$  edges. We have  $|\mathbb{A}(\mathcal{C})| = 2^m$  by Part 1 of Lemma 8.1 and  $|\mathbb{A}^*(\mathcal{C})| = 2^{m-1}$  by Part 3 of this lemma. From Lemma 7.5 it follows that  $|\mathbb{C}(\mathcal{C})| = 4^n$ . Lemma 7.4, therefore, implies that  $|\mathbb{C}_0(\mathcal{C})| = 2^{2n-m+1} = 2^{m-n+1}$ . This equality agrees with the fact, which can be derived from (47), that color-preserving automorphisms of  $\mathcal{C}$  are in one-to-one correspondence with Eulerian subgraphs of  $F_{\mathcal{C}}$ . Recall that a graph is called Eulerian if its every vertex has even degree. All Eulerian subgraphs of a connected graph with n vertices and m edges form the cycle space, which is a vector space of dimension m - n + 1 over the two-element field.

# 9 Irredundant configurations: The 3-harmonious case

# 9.1 The hypergraph of direct connections

Let  $\mathcal{C}$  be an irredundant configuration. Suppose that  $\mathcal{C}[X,Y]$  is a non-uniform interspace. We define D(X,Y) to be the set of fibers consisting of X, Y, and all Z such that  $\mathcal{C}[Z,X]$  is non-uniform and directly connected with  $\mathcal{C}[Y,X]$ . Let  $D_{\mathcal{C}}$  denote the family of all sets D(X,Y) over non-uniform interspaces  $\mathcal{C}[X,Y]$ . We regard  $D_{\mathcal{C}}$  as a hypergraph on  $F(\mathcal{C})$  and call it the hypergraph of direct connections of  $\mathcal{C}$ .

Recall that the degree of a vertex v in a hypergraph H is the number of hyperedges of H containing v. Similarly to graphs,  $\Delta(H)$  (resp.,  $\delta(H)$ ) denotes the maximum (resp., minimum) degree of a vertex in the hypergraph H. The following



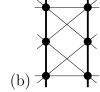


Figure 13: (a) A hypergraph of direct connections  $D_{\mathcal{C}}$  shown as a family of two 3-cliques, marked in bold, and six 2-cliques in the fiber graph  $F_{\mathcal{C}}$ . (b) A geometric representation of  $D_{\mathcal{C}}$ .

properties of irredundant configurations are known for reduced Klein configurations [31]; see also [10, Section 4.1.2]. The two classes of coherent configurations are closely related but not identical. In particular, a reduced Klein configuration cannot contain  $C_4$ -cells.

**Lemma 9.1** (cf. [10, Lemma 4.1.18]).

- **1.**  $1 \leq \delta(D_{\mathcal{C}}) \leq \Delta(D_{\mathcal{C}}) \leq 3$ . Moreover, every edge  $\{X,Y\}$  of  $F_{\mathcal{C}}$  can be extended to a hyperedge of  $D_{\mathcal{C}}$ .
- **2.** Every hyperedge of  $D_{\mathcal{C}}$  is a clique in  $F_{\mathcal{C}}$ , and all interspace connections within this clique are direct.
- **3.** Any two hyperedges of  $D_{\mathcal{C}}$  have at most one common vertex.

*Proof.* Part 1 follows from the definitions and the obvious fact that a cell contains at most three matchings where interspaces can be directly connected to each other. Lemma 5.3 implies that, if A and B are two fibers in D(X,Y), then the interspace C[A,B] is non-uniform and D(A,B) = D(X,Y). This yields Parts 2 and 3.

Lemma 9.1 shows that  $D_{\mathcal{C}}$  is a clique edge partition of  $F_{\mathcal{C}}$ . This implies that the fiber graph is reconstructable from the hypergraph of direct connections. Indeed,  $F_{\mathcal{C}}$  is the Gaifman graph of  $D_{\mathcal{C}}$ , that is, two fibers are adjacent in  $F_{\mathcal{C}}$  if and only if they are both contained in some hyperedge of  $D_{\mathcal{C}}$ .

Part 3 of Lemma 9.1 says exactly that  $D_{\mathcal{C}}$  is a linear hypergraph. Linear hypergraphs with each hyperedge of size at least 2 are known in incidence geometry [13, 30] as partial linear spaces. Here vertices of a hypergraph are interpreted as points and hyperedges as lines; see Figure 13, though not every partial linear space admits a geometric realization. A relationship between reduced Klein configurations and partial linear spaces was noticed in [10, Corollary 4.1.19]. Lemma 9.3 below shows that, under certain conditions, a coherent configuration is uniquely determined by its hypergraph of direct connections, and that partial linear spaces are a rich source of templates for constructing coherent configurations. The following elementary fact will be useful in the proof of Lemma 9.3 and also later.

### Lemma 9.2.

- 1. Let  $M_1, M_2, M_3$  be the three matching relations on a 4-element set X numbered in an arbitrary order. Then there is a permutation  $\phi$  of X such that  $\phi(M_1) = M_1$ ,  $\phi(M_2) = M_3$ , and  $\phi(M_3) = M_2$ .
- **2.** Let  $M_1$ ,  $M_2$ ,  $M_3$  be the three matching relations on a 4-element set X and  $M'_1$ ,  $M'_2$ ,  $M'_3$  be the three matching relations on a 4-element set X', numbered in an arbitrary order. Then there is a bijection  $\psi$  from X onto X' such that  $\psi(M_i) = M'_i$  for each i = 1, 2, 3.

*Proof.* Part 1 is straightforward; cf. the discussion in Section 7.1. Part 2 easily follows from Part 1.  $\Box$ 

Recall that a hypergraph is called *connected* if its Gaifman graph is connected.

#### Lemma 9.3.

- **1.** Let C be an irredundant configuration. If  $C \cong_{alg} C'$ , then  $D_C \cong D_{C'}$ , where  $\cong$  denotes isomorphism of hypergraphs.
- **2.** Under the condition  $\delta(D_{\mathcal{C}}) \geq 2$ ,  $D_{\mathcal{C}} \cong D_{\mathcal{C}'}$  implies that  $\mathcal{C} \cong_{comb} \mathcal{C}'$ .
- **3.** For any connected partial linear space D with  $\Delta(D) \leq 3$  there is an irredundant configuration C such that  $D_C \cong D$ .
- *Proof.* 1. This part follows from the fact that an algebraic isomorphism respects fibers, non-uniformity of interspaces, and direct connections of interspaces.
- 2. Let  $h: F(\mathcal{C}) \to F(\mathcal{C}')$  be an isomorphism from the hypergraph  $D_{\mathcal{C}}$  to the hypergraph  $D_{\mathcal{C}'}$ . Based on h, we define a bijection  $\bar{h}$  from the set of all matching basis relations of  $\mathcal{C}$  to the set of all matching basis relations of  $\mathcal{C}'$ . Consider a fiber  $X \in F(\mathcal{C})$ . Let  $C_1$  and  $C_2$  be two hyperedges of  $D_{\mathcal{C}}$  containing X. All interspaces  $\mathcal{C}[Y,X]$  for  $Y \in C_1$  determine the same matching in the cell  $\mathcal{C}[X]$ , which we denote by  $M_1$ . All interspaces  $\mathcal{C}[Y,X]$  for  $Y \in C_2$  determine a matching  $M_2$ , different from  $M_1$ . Thus,  $\mathcal{C}[X] \cong F_4$ . Denote the third matching in  $\mathcal{C}[X]$  by  $M_3$ . Similarly, the interspaces  $\mathcal{C}'[Y',h(X)]$  for  $Y' \in h(C_1)$  determine a matching  $M'_1$ , and the interspaces  $\mathcal{C}'[Y',h(X)]$  for  $Y' \in h(C_2)$  determine a matching  $M'_2 \neq M'_1$  in  $\mathcal{C}'[h(X)]$ . Denote the third matching in  $\mathcal{C}'[h(X)]$  by  $M'_3$  and set  $h(M_i) = M'_i$  for i = 1, 2, 3. Let  $\psi_X$  be a bijection from X onto h(X) such that  $\psi_X(M) = h(M)$  for each matching M in  $\mathcal{C}[X]$ . Such a bijection exists by Part 2 of Lemma 9.2. Combining all  $\psi_X$  over  $X \in F(\mathcal{C})$ , we obtain a bijection from  $V(\mathcal{C})$  onto  $V(\mathcal{C}')$  which is a combinatorial isomorphism from  $\mathcal{C}$  to  $\mathcal{C}'$ .
- 3. Given D, we construct  $\mathcal{C}$  as follows. Each point p of D gives rise to a 4-point fiber  $X_p$  in  $\mathcal{C}$ , with the cell  $\mathcal{C}[X_p]$  being of type  $F_4$ . With each hyperedge C of D containing p, we associate a matching relation  $M_{p,C}$  in  $\mathcal{C}[X_p]$  such that  $M_{p,C} \neq M_{p,C'}$  if  $C \neq C'$ . For each pair of points p and q in the same hyperedge C, we make the interspace  $\mathcal{C}[X_p, X_q]$  non-uniform so that it determines the matching  $M_{p,C}$  in  $\mathcal{C}[X_p]$  and the matching  $M_{q,C}$  in  $\mathcal{C}[X_q]$ .

Without the assumption  $\delta(D_{\mathcal{C}}) \geq 2$  in Part 2 of Lemma 9.3, a coherent configuration  $\mathcal{C}$  cannot be uniquely reconstructed from  $D_{\mathcal{C}}$  because, if a fiber X has degree 1 in  $D_{\mathcal{C}}$ , then the cell  $\mathcal{C}[X]$  can be not only of type  $F_4$  but also of type  $C_4$  or  $\vec{C}_4$ .

Note that  $\mathcal{C}$  is skew-connected exactly when  $|\mathcal{C}| = 2$  for all  $\mathcal{C} \in \mathcal{D}_{\mathcal{C}}$ , that is,  $\mathcal{D}_{\mathcal{C}}$  is just the edge set of the graph  $F_{\mathcal{C}}$ . Part 2 of Lemma 9.3, therefore, implies that, if  $\mathcal{C}$  is a skew-connected coherent configuration with  $\delta(F_{\mathcal{C}}) \geq 2$ , then the isomorphism  $\mathcal{C} \cong_{comb} \mathcal{C}'$  is equivalent to the isomorphism  $F_{\mathcal{C}} \cong F_{\mathcal{C}'}$ .

Remark 9.4. Curiously, Lemma 9.3 reveals a connection between irredundant coherent configurations and the multipede graphs introduced by Neuen and Schweitzer in [32]. Let  $\mathcal{C}$  be an irredundant configuration and assume for the hypergraph of direct connections of  $\mathcal{C}$  that  $\delta(D_{\mathcal{C}}) = 3$ . Consistently with the notation in [32], denote the incidence graph of the hypergraph  $D_{\mathcal{C}}$  by G = G(V, W), where  $V = F(\mathcal{C})$  is the vertex set of  $D_{\mathcal{C}}$ , i.e., the set of all fibers of  $\mathcal{C}$ , and W is the set of the hyperedges of  $D_{\mathcal{C}}$ , i.e., the cliques of directly connected fibers. Two vertices  $v \in V$  and  $w \in W$  are adjacent in G if v belongs to w. Thus, every vertex in v has degree 3 in v0. Any such bipartite graph v0 determines a multipede graph denoted in [32] by v0. This is a vertex-colored graph with vertex classes of size 4 and 2. Since we started from an irredundant configuration v0, the coloring of v0 is not refinable by 2-WL, and each color class of v0 stays as a fiber in the coherent closure v0. Let v0 be the coherent configuration obtained from v0 by cutting down all fibers of size 2 (cf. Lemma 5.1). Lemma 9.3 implies that v0 is combinatorially isomorphic to v0.

## 9.2 Separability of 3-harmonious configurations

We say that a coherent configurations C is 3-harmonious if the following three conditions are met:

- $\mathcal{C}$  is irredundant;
- Every fiber of C belongs to exactly three cliques in  $D_C$  (that is,  $D_C$  is a 3-regular hypergraph);
- |C| = 3 for all  $C \in D_{\mathcal{C}}$  (that is,  $D_{\mathcal{C}}$  is a 3-uniform hypergraph).

If C is 3-harmonious, then the incidence graph of the hypergraph  $D_C$  is a cubic bipartite graph, which readily implies the equality

$$|D_{\mathcal{C}}| = |F(\mathcal{C})|. \tag{49}$$

**Lemma 9.5.** If C is 3-harmonious, then  $f_S \in A(C)$  exactly in the following case: For each clique  $C \in D_C$ , the switch set S contains two or no edges of C.

*Proof.* ( $\Longrightarrow$ ) Suppose that  $C \in D_{\mathcal{C}}$  and  $C = \{X, Y, Z\}$ . If  $f_S \in \mathbb{A}(\mathcal{C})$ , then the restriction of  $f_S$  to  $\mathcal{C}[X \cup Y \cup Z]$  is a strict automorphism of this subconfiguration. By Part 2 of Lemma 7.6,  $f_S$  is either identity on  $\mathcal{C}[X \cup Y \cup Z]$  or switches exactly two edges of C.

$$(\Leftarrow)$$
 This part follows directly from Lemma 7.6 by Lemma 3.4.

**Lemma 9.6.** A 3-harmonious coherent configuration C is separable if and only if the group of color-preserving automorphisms  $\mathbb{C}_0(C)$  is trivial.

Proof. Lemma 9.5 implies that

$$|\mathbb{A}(\mathcal{C})| = 4^{|D_{\mathcal{C}}|}.$$

Since every cell of a 3-harmonious coherent configuration is of type  $F_4$ , Lemma 7.5 implies that  $\mathbb{C}(\mathcal{C}) \cong \prod_{X \in F(\mathcal{C})} K(X)$  and, therefore,

$$|\mathbb{C}(\mathcal{C})| = 4^{|F(\mathcal{C})|}.$$

Taking into account Equality (49), we conclude by Lemma 7.4 that  $\mathbb{A}^*(\mathcal{C}) = \mathbb{C}(\mathcal{C})$  if and only if  $|\mathbb{C}_0(\mathcal{C})| = 1$ .

Lemma 9.6 provides an efficient separability test for 3-harmonious coherent configurations. Given a 3-harmonious coherent configuration  $\mathcal{C}$ , we construct a vertex colored graph  $G(\mathcal{C}) = G$  as follows:

- V(G) = V(C).
- The vertex color classes of G are exactly the fibers of C.
- $\bullet$  Every vertex color class of G is an independent set.
- For two disjoint sets X and Y of vertices of G, let G[X, Y] denote the subgraph of G on the vertex set  $X \cup Y$  formed by the edges between a vertex in X and a vertex in Y. For each non-uniform interspace  $\mathcal{C}[X,Y]$ , we set G[X,Y] to be one of the two  $2K_{2,2}$  graphs underlying the basis relations of  $\mathcal{C}[X,Y]$ . We do not specify which of the two relations in  $\mathcal{C}[X,Y]$  shall be used to construct G[X,Y] as this is irrelevant for our purpose.

Note that  $\phi$  is a color-preserving automorphism of  $\mathcal{C}$  exactly when  $\phi$  is an automorphism of  $G(\mathcal{C})$ . Since  $G(\mathcal{C})$  has color multiplicity 4, whether it has a non-trivial automorphism is efficiently verifiable by the known techniques [1, 29].

We now show that there exist 3-harmonious coherent configurations of both sorts — separable and non-separable. Recall that the hypergraph of direct connections  $D_{\mathcal{C}}$  can be viewed as a partial linear space. Moreover, if  $\mathcal{C}$  is 3-harmonious, then every line contains exactly 3 points and every point is incident to exactly 3 lines. Partial linear spaces with n points having these properties are known as  $(n_3)$ -configurations; see [19, 34]. Lemma 9.3 implies a one-to-one correspondence between  $(n_3)$ -configurations and 3-harmonious coherent configurations with n fibers.

There is no  $(n_3)$ -configuration for  $n \leq 6$ . There are a unique  $(7_3)$ -configuration, namely the *Fano plane*, and a unique  $(8_3)$ -configuration, namely the *Möbius-Kantor configuration*; see Figure 14. We denote the corresponding 3-harmonious coherent configurations by  $\mathcal{C}_{\text{Fano}}$  and  $\mathcal{C}_{\text{MK}}$  respectively.

**Theorem 9.7.**  $\mathcal{C}_{Fano}$  is non-separable, and  $\mathcal{C}_{MK}$  is separable.

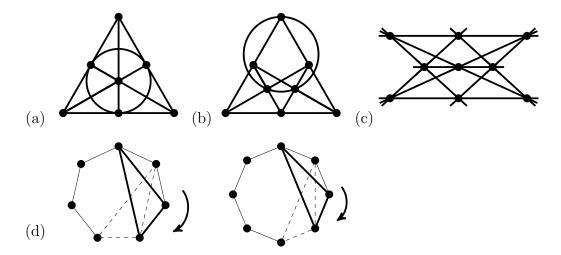


Figure 14: (a) The Fano plane. (b) The Möbius-Kantor configuration. One 3-point "line" in (a) and in (b) is drawn as a circle. (c) The Pappus configuration. (d) Construction of the cyclic versions  $D_7$  and  $D_8$  of the Fano and the Möbius-Kantor configurations.

In fact, we prove a more general fact. Let  $n \geq 7$ . The cyclic  $(n_3)$ -configuration  $D_n$  is constructed as follows [19, Section 2.1]. Let  $F_n$  be the Cayley graph of  $\mathbb{Z}_n$  with the difference set  $\{\pm 1, \pm 2, \pm 3\}$  and  $D_n$  be the hypergraph formed by 3-cliques  $\{i, i+2, i+3\}$  in  $F_n$ , where  $i \in \mathbb{Z}_n$ . It is straightforward to see that  $D_n$  is really an  $(n_3)$ -configuration. By the uniqueness of  $(n_3)$ -configurations for n=7,8 (see, e.g., [34, Theorem 5.13]), the Fano plane is isomorphic, as a hypergraph, to  $D_7$ , and the Möbius-Kantor configuration is isomorphic to  $D_8$ . Let  $C_n$  be the coherent configuration constructed from  $D_n$  as in the proof of Part 3 of Lemma 9.3. This lemma implies that  $C_{\text{Fano}} \cong_{comb} C_7$  and  $C_{\text{MK}} \cong_{comb} C_8$ . Thus, Theorem 9.7 is equivalent to the statement that  $C_n$  is non-separable if n=7 and separable if n=8.

**Theorem 9.8.** Let  $n \geq 7$ . The coherent configuration  $C_n$  is non-separable if and only if n is a multiple of 7.

*Proof.* Fix a vertex-colored graph  $G_n = G(\mathcal{C}_n)$  as described above. By Lemma 9.6, it suffices to show that  $G_n$  has a non-trivial automorphism if and only if n is divisible by 7. Recall that the graph  $G_n$  is not uniquely determined (not even up to isomorphism). It can be constructed in many non-isomorphic ways, and any variant is suitable for our purposes (as the automorphism group of  $G_n$  always coincides with  $\mathbb{C}_0(\mathcal{C}_n)$ , that is, is the same for any particular implementation of the construction). To fix the notation, we turn back to construction of  $\mathcal{C}_n$  from  $D_n$  and make some specifications.

Specifically, we set  $V(\mathcal{C}_n) = \{(i,j) : i \in \mathbb{Z}_n, 1 \leq j \leq 4\}$ . The fibers of  $\mathcal{C}_n$  are the sets  $X_i = \{(i,1), (i,2), (i,3), (i,4)\}$  for each  $i \in \mathbb{Z}_n$  and, correspondingly, each vertex from  $X_i$  has color i in  $G_n$ . From now on, we will just refer to (i,j) as the vertex j in color class  $X_i$ , i.e., drop the (i,j) in most cases. Recall that the construction ensures that  $\mathcal{C}[X_i] \simeq F_4$ . Let M, N, L be the three matching relations in  $\mathcal{C}[X_i]$ .

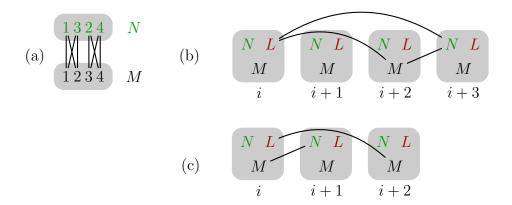


Figure 15: (a) The subgraph  $G_n[X_{i+2}, X_{i+3}]$  corresponds to the  $2K_{2,2}$ -interspace  $C_n[X_{i+2}, X_{i+3}]$ , determining the matchings M in  $C_n[X_{i+2}]$  and N in  $C_n[X_{i+3}]$ . (b) The constraints on an automorphism  $\phi$  of  $G_n$  imposed by the triangle  $\{i, i+2, i+3\}$  in  $D_n$ . (c) The two constraints on  $\phi_i$ ,  $\phi_{i+1}$ , and  $\phi_{i+2}$  involving  $\phi_i$ .

For each  $i \in \mathbb{Z}_n$ , the triangle  $\{i, i+2, i+3\}$  in  $D_n$  contributes a triple of directly connected non-uniform interspaces in  $\mathcal{C}_n$ . We construct  $\mathcal{C}_n$  so that the non-uniform interspaces  $\mathcal{C}_n[X_i, X_{i+2}]$ ,  $\mathcal{C}_n[X_i, X_{i+3}]$ , and  $\mathcal{C}_n[X_{i+2}, X_{i+3}]$  determine the matchings L in  $\mathcal{C}_n[X_i]$ , M in  $\mathcal{C}_n[X_{i+2}]$ , and N in  $\mathcal{C}_n[X_{i+3}]$ ; see Figure 15(a). This defines the coherent configuration  $\mathcal{C}_n$  unambiguously; cf. Lemma 9.3. Figure 15(b) shows the connection scheme of the above three interspaces, which is the same for each  $i \in \mathbb{Z}_n$ . In the graph  $G_n = G(\mathcal{C}_n)$ , there remain two possibilities for each of the subgraphs  $G_n[X_i, X_{i+2}]$ ,  $G_n[X_i, X_{i+3}]$ , and  $G_n[X_{i+2}, X_{i+3}]$ , but for the following argument it does not matter which  $2K_{2,2}$ -fragment is in the graph and which is in its complement. We make an arbitrary choice in each case, and  $G_n$  is therewith fixed.

Let  $\phi$  be an automorphism of  $G_n$ , and let  $\phi_i$  denote the restriction of  $\phi$  to  $X_i$ . Since  $\phi_i$  must map each matching of  $X_i$  onto itself, this permutation belongs to the Klein four-group  $K(X_i)$  consisting of the permutations  $\psi_0 = \mathrm{id}_{X_i}$ ,  $\psi_M = (12)(34)$ ,  $\psi_N = (13)(24)$  and  $\psi_L = (14)(23)$ . Differently from the terminology after Lemma 7.5, we now name the non-identity group elements by the matching relation they fix, e.g.,  $\psi_M = \phi_{NL}$ .

The three connections between matchings shown in Figure 15(b) can be seen as constraints on a sequence  $(\phi_j)_{j\in\mathbb{Z}_n}$  corresponding to an automorphism  $\phi$ . Indeed, if  $\phi$  fixes (resp. flips) one of the three connected matchings, then it must also fix (resp. flip) each of the other two. For example, if  $\phi_i = \psi_L$ , then  $\phi_{i+2}$  must fix the matching M on  $X_{i+2}$ , which implies that either  $\phi_{i+2} = \psi_M$  or  $\phi_{i+2} = \psi_0$ , where  $\psi_0 = \mathrm{id}_{X_{i+2}}$ . Figure 15(c) shows the two constraints on  $\phi_i$  and the two subsequent local automorphisms  $\phi_{i+1}$  and  $\phi_{i+2}$ . Alternatively these constraints can be described by a table in Table 1(a). Consider, for example, the first row of this table, which corresponds to the equality  $\phi_i = \psi_M$ . The constraint on the pair  $(\phi_i, \phi_{i+1})$  forces  $\phi_{i+1}$  to fix the matching N and, therefore,  $\phi_{i+1} \in \{\psi_N, \psi_0\}$ . Furthermore, since  $\phi_i = \psi_M$  flips L, the constraint on the pair  $(\phi_i, \phi_{i+2})$  forces  $\phi_{i+2}$  to flip M and,

therefore,  $\phi_{i+2} \in \{\psi_N, \psi_L\}$ . Table 1(a) gives eight possibilities for the pair  $(\phi_i, \phi_{i+1})$ . It turns out that, in each of these eight cases, Table 1(a) determines the next local automorphism  $\phi_{i+2}$  unambiguously. This can be seen from Table 1(b). For example, if  $\phi_i = \psi_M$ , then column i+2 of Table 1(a) shows that  $\phi_{i+2} \in \{\psi_N, \psi_L\}$ . If, moreover,  $\phi_{i+1} = \psi_N$ , then the intersection of column i+1 and row N of Table 1(a) shows that  $\phi_{i+2} \in \{\psi_M, \psi_L\}$ . Therefore, the equalities  $\phi_i = \psi_M$  and  $\phi_{i+1} = \psi_N$  imply that  $\phi_{i+2} = \psi_L$ .

					i	i+1	i+2		i+3
					M	N	L	$= \{N, L\} \cap \{M, L\}$	L
	i	i+1	i+2		M	0	N	$= \{N, L\} \cap \{0, N\}$	M
	M	0/N	N/L		N	M	N	$= \{N, L\} \cap \{0, N\}$	L
(a)	N	M/L	N/L	(b)	N	L	L	$= \{N, L\} \cap \{M, L\}$	M
	L	M/L	0/M		L	M	0	$= \{0, M\} \cap \{0, N\}$	N
	0	0/N	0/M		L	L	M	$= \{0, M\} \cap \{M, L\}$	0
					0	N	M	$= \{0, M\} \cap \{M, L\}$	N
					0	0	0	$= \{0, M\} \cap \{0, N\}$	0

Table 1: (a) A table representation of the constraints on  $\phi_i$  and  $\phi_{i+1}$  and on  $\phi_i$  and  $\phi_{i+2}$  depicted in Figure 15(c). (b) Extrapolation of the sequence  $(\phi_i)_i$  on the basis of  $\phi_i$ ,  $\phi_{i+1}$  and the recurrence relation implied by Table (a).

The rest of our analysis is based on Table 1(b). Observe that the eight pairs in columns i and i+1 are exactly the same as the eight pairs in columns i+1 and i+2. It follows that the constraints of Table (a) completely determine the entire sequence  $(\phi_j)_j$  for each of the eight consistent pairs  $(\phi_i, \phi_{i+1})$ , for an arbitrarily fixed i. We can imagine that the index j ranges through the set of all integers, remembering that it has to be considered modulo n. Moreover, observe that the pair (0,0) stays in the same row, while the other seven pairs  $(M,N),\ldots,(0,N)$  change their rows according to the cyclic permutation (1372564). This has the following consequences. First, the pair (M,N) eventually appears in every non-zero row and, hence, the infinite expansions of the seven non-zero rows are identical up to a shift. Second, the sequence that appears in this way is periodic with period 7. It follows that, if  $G_n$  has a nontrivial automorphism  $\phi$ , then the corresponding infinity sequence of local automorphisms  $(\phi_j)_j$ , where each index j is considered modulo n, must be periodic with period 7, namely

$$\dots \quad \phi_i \quad \phi_{i+1} \quad \phi_{i+2} \quad \phi_{i+3} \quad \phi_{i+4} \quad \phi_{i+5} \quad \phi_{i+6} \quad \dots \\
\dots \quad \psi_M \quad \psi_N \quad \psi_L \quad \psi_L \quad \psi_M \quad \psi_0 \quad \psi_N \quad \dots$$
(50)

for some choice of i. We immediately conclude from here that, if n is not divisible by 7, then  $G_n$  has no nontrivial automorphism.

Table 1(b) includes also column i+3. Looking at columns i and i+3, we see that, in each of the eight possible cases,  $\phi_{i+3}$  fixes N whenever  $\phi_i$  fixes L, and  $\phi_{i+3}$  flips N whenever  $\phi_i$  flips L. This leads us to the following conclusion: If a sequence  $(\phi_i)_i$ 

satisfies the constraints on  $\phi_i$  and  $\phi_{i+2}$  and  $\phi_{i+2}$  and  $\phi_{i+3}$ , shown in Figure 15(b), for every i, then it also satisfies the constraint on  $\phi_i$  and  $\phi_{i+3}$  for every i. It readily follows that, if n is divisible by 7, then any assignment of local automorphisms as in (50) determines a nontrivial automorphism  $\phi$  of  $G_n$ .

**Remark 9.9.** There are exactly three  $(9_3)$ -configurations [19, 34]. The most famous of them is the *Pappus configuration* shown in Figure 14(c). Computer-assisted verification shows that the corresponding 36-point coherent configuration is non-separable. Of the other two  $(9_3)$ -configurations, one is the cyclic  $(9_3)$ -configuration defined above, and the other is obtained similarly by rotating the triangle  $\{0, 3, 4\}$  (instead of  $\{0, 2, 3\}$ ) in  $\mathbb{Z}_9$ . These two produce separable coherent configurations.

# 10 Irredundant configurations: The general case

Given  $C \in D_{\mathcal{C}}$  and a non-empty  $U \subsetneq C$ , let S(U,C) be the set of all edges  $\{X,Y\}$  in  $F_{\mathcal{C}}$  such that  $X \in U$  and  $Y \in C \setminus U$ . Using the notation  $f_S$  introduced in Section 7.1, we now define  $f_{X,C} = f_{S(\{X\},C)}$  for  $X \in C$ ,.

**Lemma 10.1.** Suppose that a coherent configuration C is irredundant.

- **1.**  $f_S \in \mathbb{A}(\mathcal{C})$  if and only if, for every  $C \in D_{\mathcal{C}}$ , either the intersection  $S \cap \binom{C}{2}$  is empty or it forms a spanning bipartite subgraph of  $\binom{C}{2}$ , where  $\binom{C}{2}$  is considered the complete graph on the vertex set C.
- **2.**  $\mathbb{A}(\mathcal{C})$  is generated by the set of  $f_{X,C}$  for all  $C \in D_{\mathcal{C}}$  and all  $X \in C$ .

*Proof.* 1. For  $C \in D_{\mathcal{C}}$ , denote  $S[C] = S \cap {C \choose 2}$ . By Lemma 9.1,  $\{S[C]\}_{C \in D_{\mathcal{C}}}$  is a partition of S. Therefore,

$$f_S = \prod_{C \in D_C} f_{S[C]}. \tag{51}$$

- ( $\Leftarrow$ ) It suffices to prove that each  $f_{S[C]}$  is an algebraic automorphism of  $\mathcal{C}$ . By Lemma 3.4, it is enough to check that, for every triple of fibers X,Y,Z, the restriction of  $f_{S[C]}$  to  $\mathcal{C}[X \cup Y \cup Z]$  is an algebraic automorphism of  $\mathcal{C}[X \cup Y \cup Z]$ . If  $|\{X,Y,Z\} \cap C| \leq 1$ , then  $f_{S[C]}$  is the identity on  $\mathcal{C}[X \cup Y \cup Z]$ . If  $|\{X,Y,Z\} \cap C| = 2$ , then Lemma 5.3 implies that  $\mathcal{C}[X \cup Y \cup Z]$  is either decomposable or skew-connected. The former case is obvious, and in the latter case we are done by Part 1 of Lemma 7.6. If  $\{X,Y,Z\} \subseteq C$ , then the bipartiteness of S[C] implies that  $f_{S[C]}$  switches either two (up to transposing) or no interspaces between X,Y,Z. In this case we are done by Part 2 of Lemma 7.6.
- $(\Longrightarrow)$  Let  $C \in D_{\mathcal{C}}$  and suppose that S[C] is non-empty. The claim is trivially true if |C| = 2, so we assume that  $|C| \ge 3$ . Let X, Y, and Z be three fibers in C. By assumption, the restriction of  $f_S$  to  $C[X \cup Y \cup Z]$  is an algebraic automorphism of  $C[X \cup Y \cup Z]$ . By Part 2 of Lemma 7.6,  $f_S$  makes either none or exactly two switches in  $C[X \cup Y \cup Z]$ . For S[C], seen as a graph on the vertex set C, this implies that S[C] does not contain any induced subgraph isomorphic to  $K_3$  or to  $K_2 + K_1$ ,

where the latter is the graph with 3 vertices and 1 edge. A graph is  $(K_2 + K_1)$ -free if and only if it is complete multipartite. To see this, look at the complement and note that a graph is a vertex-disjoint union of cliques if and only if it does not contain an induced copy of a path on 3 vertices, the complement of  $K_2 + K_1$ . Thus, S[C] is a complete multipartite graph. Since S[C] is also triangle-free, it is bipartite.

2. By Equality (51), Part 1 implies that  $\mathbb{A}(\mathcal{C})$  is generated by the set of  $f_{S(U,C)}$  for all  $C \in D_{\mathcal{C}}$  and  $\emptyset \neq U \subsetneq C$ . Note that, if U is split into two non-empty parts  $U_1$  and  $U_2$ , then  $f_{S(U,C)} = f_{S(U_1,C)} \circ f_{S(U_2,C)}$  (as each interspace between  $U_1$  and  $U_2$  is switched twice). It follows that

$$f_{S(U,C)} = \prod_{X \in U} f_{X,C},$$

which implies the lemma.

Lemma 10.1 suggests two approaches to deciding separability of an irredundant configuration.

**1st approach** is based on Part 1 of Lemma 10.1. We infer from it that

$$|\mathbb{A}(\mathcal{C})| = \prod_{C \in D_{\mathcal{C}}} 2^{|C|-1} = 2^{\left(\sum_{C \in D_{\mathcal{C}}} |C|\right) - |D_{\mathcal{C}}|}.$$
 (52)

It remains to compute the order of the group  $\mathbb{A}^*(\mathcal{C})$  and check whether or not  $|\mathbb{A}^*(\mathcal{C})| = |\mathbb{A}(\mathcal{C})|$ . By Lemma 7.4,  $|\mathbb{A}^*(\mathcal{C})| = |\mathbb{C}(\mathcal{C})|/|\mathbb{C}_0(\mathcal{C})|$ , where  $|\mathbb{C}(\mathcal{C})|$  is easy to determine using Lemma 7.5. Indeed, Lemma 7.5 says that  $\mathbb{C}(\mathcal{C}) \cong \prod_{X \in F(\mathcal{C})} \mathbb{C}_0(\mathcal{C}[X])$ , and we have  $\mathbb{C}_0(\mathcal{C}[X]) = K(X)$  (the Klein group of order 4) for  $\mathcal{C}[X] \simeq F_4$ ,  $\mathbb{C}_0(\mathcal{C}[X]) \cong \mathbb{D}_4$  (the dihedral group of order 8) for  $\mathcal{C}[X] \simeq C_4$ , and  $\mathbb{C}_0(\mathcal{C}[X]) \cong \mathbb{Z}_4$  (the cyclic group of order 4) for  $\mathcal{C}[X] \simeq \vec{C}_4$ . It remains to compute the order of the group of color-preserving automorphisms  $|\mathbb{C}_0(\mathcal{C})|$ . To this end, we construct a vertex-colored graph  $G^*(\mathcal{C})$  whose automorphism group  $\mathrm{Aut}(G^*(\mathcal{C}))$  is precisely  $\mathbb{C}_0(\mathcal{C})$ , compute a set of generators of  $\mathrm{Aut}(G^*(\mathcal{C}))$  as in [1], and apply the Schreier-Sims algorithm to compute the order of  $\mathrm{Aut}(G^*(\mathcal{C}))$  based on this set of generators.

We construct  $G^* = G^*(\mathcal{C})$  similarly to the graph  $G(\mathcal{C})$  in Section 9 with the only difference that, for each  $X \in F(\mathcal{C})$ , the subgraph  $G^*[X]$  induced by  $G^*$  on X is defined more carefully:

- If there are interspaces C[Y, X] and C[Z, X] with askew connection at X, then  $G^*[X]$  is empty (in this case  $C[X] \simeq F_4$  by Part 2 of Lemma 5.2, and each matching relation on X will be anyway preserved by any automorphism of  $G^*$ );
- Otherwise,  $G^*[X]$  depends on  $\mathcal{C}[X]$ . We define  $G^*[X]$  so that  $\operatorname{Aut}(G^*[X])$  consists exactly of the color-preserving combinatorial automorphisms of  $\mathcal{C}[X]$  (i.e., those mapping each basis relation of  $\mathcal{C}[X]$  onto itself). Specifically,

- if  $C[X] \simeq F_4$ , then we put a matching  $2K_2$  in  $G^*[X]$  different from the one determined by some interspace C[Y, X] (at least one such an interspace must exist because C is indecomposable);
- if  $C[X] \simeq C_4$ , then we leave  $G^*[X]$  empty (a matching on X is implicitly determined anyway);
- if  $C[X] \simeq \vec{C}_4$ , we have to put a directed 4-cycle in  $G^*[X]$  coherently with the matching implicitly determined on X. To avoid making  $G^*$  a directed graph, we subdivide each edge of this cycle with two differently colored vertices in the direction given by  $\vec{C}_4$ . This costs us two new colors and four new vertices of each of these colors (which we put in  $V(G^*)$  in addition to the vertices of C).

**2nd approach** is based on Part 2 of Lemma 10.1. For each pair (X, C) where  $X \in C \in D_{\mathcal{C}}$ , we check whether the algebraic automorphism  $f_{X,C}$  is induced by a combinatorial automorphism. A crucial fact is that the number of such pairs is polynomially bounded. Fix  $G^* = G^*(\mathcal{C})$  as above and obtain a graph  $G^*_{X,C}$  from  $G^*$  by complementing each bipartite subgraph  $G^*[X,Y]$  spanned by the fiber X and a fiber Y in  $C \setminus \{X\}$ . By construction, a combinatorial automorphism  $\phi$  of  $\mathcal{C}$  induces  $f_{X,C}$  exactly when  $\phi$  is an isomorphism of the graphs  $G^*$  and  $G^*_{X,C}$ . Thus,  $f_{X,C}$  is induced by a combinatorial automorphism if and only if  $G^* \cong G^*_{X,C}$ . The last condition is efficiently verifiable [1] as the graphs  $G^*$  and  $G^*_{X,C}$  are of color multiplicity 4.

Remark 10.2. Following the second approach, instead of  $G^* = G^*(\mathcal{C})$  we can still use the simpler construction  $G = G(\mathcal{C})$  exactly as described in Section 9 (where G[Z] for each  $Z \in F(\mathcal{C})$  is an independent set). Though the automorphism group  $\operatorname{Aut}(G(\mathcal{C}))$  can be strictly larger than  $\mathbb{C}_0(\mathcal{C})$ , it is easy to see that  $G \cong G_{X,C}$  exactly when  $G^* \cong G^*_{X,C}$ . Indeed, any isomorphism  $\phi$  from  $G^*$  to  $G^*_{X,C}$  is obviously an isomorphism also from G to  $G_{X,C}$ . Conversely, let  $\phi$  be an isomorphism from G to  $G_{X,C}$ . Suppose that  $\mathcal{C}[Z]$  is a cell with a single determined matching M. Any modification  $\phi^*$  of  $\phi$  within Z which maps M onto itself and flips M if and only if  $\phi$  does so stays an isomorphism from G to  $G_{X,C}$ . It follows that  $\phi$  admits a modification  $\phi^*$  such that  $\phi^*$  is not only an isomorphism from G to  $G_{X,C}$  but also an automorphism of  $G^*[Z]$ . Making such a modification on each such fiber Z, we obtain an isomorphism  $\phi^*$  from  $G^*$  to  $G^*_{X,C}$ . Summarizing, we see that our decision procedure has the same outcome regardless of whether the simpler construction  $G(\mathcal{C})$  or its augmented version  $G^*(\mathcal{C})$  is used.

**Example 10.3.** We make use of the construction of a coherent configuration C = C(D) based on a given partial linear space D as described in the proof of Part 3 of Lemma 9.3. For the partial linear space D depicted in Figure 13(a), the coherent configuration C(D) is separable. By Part 2 of Lemma 10.1, it is enough to show that each  $f_{X,C}$  is induced by a combinatorial automorphism. Suppose first that |C| = 3, say,  $C = \{X, Y, Z\}$ . For appropriate combinatorial automorphisms  $\phi \in K(Y)$  and

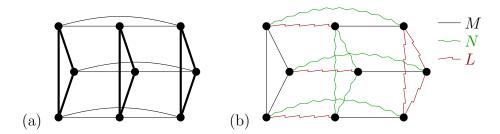


Figure 16: (a) A pattern D is represented as a clique partition of a 9-vertex graph consisting of three 3-cliques and nine 2-cliques. (b) We can assign the names M, N and L to the matching basis relations of each cell in  $\mathcal{C}(D)$  such that every interspace connects matchings with the same name. Each edge color in the depicted graph represents this name.

 $\psi \in K(Z)$ , we have  $\phi \psi f_{X,C} = f_S$  where S consists of two edges of  $F_C$  emanating from Y and Z such that each of them forms a 2-clique in  $D = D_C$ . Note that the six edges of this kind form a connected subgraph of  $F_C$ . Like the analysis of the CFI case in Section 8, we see that  $f_S$  is induced by a combinatorial automorphism. Since  $f_{X,C} = \psi^{-1}\phi^{-1}f_S$ , the same holds true for  $f_{X,C}$ .

Suppose now that |C| = 2, say,  $C = \{X, Y\}$ . Let C' be the hyperedge of D such that  $X \in C'$  and |C'| = 3. For a suitable combinatorial automorphisms  $\phi \in K(X)$ , we have  $\phi f_{X,C} = f_{X,C'}$ . We already know that  $f_{X,C'}$  is induced by a combinatorial automorphism. Therefore, this is so also for  $f_{X,C} = \phi^{-1} f_{X,C'}$ .

Consider the same example also from the perspective of Part 1 of Lemma 10.1. By Equality (52), we have  $|\mathbb{A}(\mathcal{C})| = 2^{10}$ . As it readily follows from Lemma 7.5,  $|\mathbb{C}(\mathcal{C})| = 2^{12}$ . We already know that  $|\mathbb{A}^*(\mathcal{C})| = |\mathbb{A}(\mathcal{C})|$ , and Lemma 7.4 implies that  $|\mathbb{C}_0(\mathcal{C})| = 4$ . This can be seen also directly. Moreover,  $\mathbb{C}_0(\mathcal{C})$  is isomorphic to the Klein four-group. Indeed, let  $X_1, \ldots, X_6$  be the fibers of  $\mathcal{C}$ . If  $\phi$  is a color-preserving automorphism of  $\mathcal{C}$ , then  $\phi = \prod_{i=1}^6 \phi_i$ , where each  $\phi_i \in K(X_i)$  is extended by identity outside  $X_i$ . For every choice of a non-identity permutation  $\phi_1$ , a simple argument shows that each of the other factors  $\phi_2, \ldots, \phi_6$  is uniquely determined.

Example 10.4. Consider next D shown in Figure 16(a). This pattern yields a non-separable coherent configuration  $\mathcal{C} = \mathcal{C}(D)$ . To see this, we make use of the names M, N and L for the matching basis relations in each cell as introduced after Lemma 7.5 and assign these names as shown in Figure 16(b). Note that the nine 2-cliques in D form three disjoint 3-cycles, each with exactly one edge of the type M, N and L. Combining the local combinatorial automorphisms  $\phi_{NL}$ ,  $\phi_{ML}$  and  $\phi_{MN}$  of the three cells in such a cycle (e.g., for the cells in the top row of Figure 16(b)) we get a nontrivial combinatorial automorphism that induces a trivial algebraic automorphism, i.e., a nontrivial color-preserving combinatorial automorphism. By doing this on any one, two or three multicolored cycles, we obtain  $2^3 - 1 = 7$  nontrivial color-preserving automorphisms.

Three further such automorphisms can be constructed from the monochromatic

3-cliques. Consider, for instance, the M- and the N-cliques. They are connected by a matching consisting of three L-edges. If we pick  $\phi_{ML}$  for each cell of the M-clique and  $\phi_{NL}$  for each cell of the N-clique, we obtain a nontrivial color-preserving automorphism. The other two pairs of monochromatic 3-cliques give us two more such automorphisms. It follows that  $|\mathbb{C}_0(\mathcal{C})| \geq 10$ . By Lemma 7.5,  $|\mathbb{C}(\mathcal{C})| = 4^9 = 2^{18}$ . Lemma 7.4, therefore, implies that  $|\mathbb{A}^*(\mathcal{C})| \leq 2^{18}/10 < 2^{15}$ . On the other hand, by (52), we have  $|\mathbb{A}(\mathcal{C})| = 2^{3\cdot 3+9\cdot 2-12} = 2^{15}$ . This implies that not all strict algebraic automorphisms of  $\mathcal{C}$  are induced by combinatorial automorphisms and, thus,  $\mathcal{C}$  is non-separable.

# 11 Putting it together

We are now prepared to prove Theorem 1.1. The cut-down lemmas (that is, Lemmas 4.1, 5.1, and 6.1) and our analysis of the irredundant case in Section 7 yield the following algorithm for recognizing whether or not a given coherent configuration  $\mathcal{C}$  with fibers of size at most 4 is separable.

- Decompose C in the direct sum of indecomposable subconfigurations  $C_1, \ldots, C_m$  and handle each of them separately. By Lemma 3.2, C is separable if and only if every  $C_i$  is separable.
- Assume, therefore, that the input configuration  $\mathcal{C}$  is indecomposable. If all fibers of  $\mathcal{C}$  are of size at most 3, immediately decide that  $\mathcal{C}$  is separable (see Corollary 4.9). Otherwise:
  - Remove all fibers of size 2 from C.
  - Remove all pairs of fibers X and Y with  $\mathcal{C}[X,Y] \simeq C_8$ .
  - As long as  $\mathcal{C}$  contains an interspace  $\mathcal{C}[X,Y]$  with a matching, remove the fiber X from  $\mathcal{C}$ .
- If  $\mathcal{C}$  becomes decomposable, split it into indecomposable components and handle each of them separately.
- If  $\mathcal{C}$  becomes empty, decide that  $\mathcal{C}$  is separable.
- Otherwise, we arrive at the case that C is irredundant and proceed as described in Section 10.
- If all computational paths terminate with a positive decision, output 'C is separable'; otherwise, output 'C is non-separable'.

Due to [1], each computational path for an irredundant coherent configuration is implementable in  $\oplus L$ . A list of all subconfigurations to which this step is applied can clearly be generated in logarithmic space [35]. Since  $L^{\oplus L} = \oplus L$  (see [8]), the whole algorithm can be implemented in  $\oplus L$ . Theorem 1.1 is proved.

As a by-product of our analysis, we state the following fact.

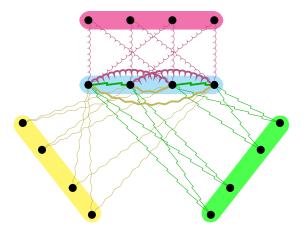


Figure 17: A fragment of the unique non-separable coherent configuration  $\mathcal{T}$  with 16 points: Three pairwise skew-connected interspaces and the matching basis relations they induce.

#### Theorem 11.1.

- 1. All coherent configurations with 15 or fewer points and maximum fiber size 4 are separable.
- 2. There is a unique, up to combinatorial isomorphism, non-separable coherent configuration on 16 points with maximum fiber size 4.

Proof. 1. Suppose that a coherent configuration has at most 15 vertices. After cutting down 2-point cells, matching interspaces, and  $C_8$ -interspaces and ignoring possible single-fiber components, we are faced with an irredundant configuration  $\mathcal{C}$  having 2 or 3 fibers. It follows from Lemma 5.3 that  $\mathcal{C}$  is either skew-connected or has 3 fibers with all connections between non-uniform fibers being direct. In the former case, since we obviously have  $\delta(F_{\mathcal{C}}) \leq 2$ , the coherent configuration  $\mathcal{C}$  is separable by Corollary 8.2. In the latter case, the separability of  $\mathcal{C}$  follows from Part 2 of Lemma 10.1. Indeed,  $D_{\mathcal{C}}$  consists of a single 3-element hyperedge C, and we only have to check that  $f_{X,\mathcal{C}}$  for any  $X \in \mathcal{C}$  is induced by a combinatorial automorphism  $\phi$ . Let M be the matching basis relation in  $\mathcal{C}[X]$  determined by the interspaces between X and the other two cells in C. As a desired  $\phi$ , we can take any color-preserving automorphism of  $\mathcal{C}[X]$  flipping M and extend it to  $V(\mathcal{C})$  by identity. Such an automorphism exists in all three cases  $\mathcal{C}[X] \simeq F_4, C_4, \vec{C}_4$  (cf. the proof of Part 2 of Lemma 8.1).

2. Taking into account the proof of Part 1, we only have to consider the case that an irredundant configuration  $\mathcal{C}$  has 4 fibers. If  $D_{\mathcal{C}}$  consists of a single 4-element hyperedge, that is, all interspaces are non-uniform and all connections between them are direct, then the separability of  $\mathcal{C}$  follows by Part 2 of Lemma 10.1 as in Part 1.

Suppose now that  $D_{\mathcal{C}}$  has a hyperedge C of size 3. To show that  $\mathcal{C}$  is separable, we again use Part 2 of Lemma 10.1. Let  $X \in C$ . Note that the degree of X in

the hypergraph  $D_{\mathcal{C}}$  is at most 2. Therefore, the same argument as in Part 1 works, showing that  $f_{X,C}$  is induced by a combinatorial automorphism of  $\mathcal{C}$ . Similarly,  $f_{X,C'}$  is induced by a combinatorial automorphism if X belongs also to a 2-element hyperedge C' of  $D_{\mathcal{C}}$ . More specifically, in this case we have  $C' = \{X,Y\}$  where Y is the fiber of  $\mathcal{C}$  not belonging to C. Thus, the interspace  $\mathcal{C}[X,Y]$  is non-uniform, and  $\mathcal{C}[X] \simeq F_4$  with one matching N determined by  $\mathcal{C}[Y,X]$  and another matching M determined by the interspaces between X and the other two fibers in C. Then  $f_{X,C'}$  is induced by  $\phi_{NL} \in K(X)$  where L is the other matching in  $\mathcal{C}[X]$  different from N and M.

If all hyperedges of  $D_{\mathcal{C}}$  are of size 2, then  $\mathcal{C}$  is skew-connected. By Corollary 8.2,  $\mathcal{C}$  is separable exactly when  $\delta(F_{\mathcal{C}}) \leq 2$ . It remains to note that  $\delta(F_{\mathcal{C}}) = 3$  in the only case that  $F_{\mathcal{C}}$  is the complete graph on 4 vertices; see Figure 17. Any two skew-connected coherent configurations with such fiber graph are combinatorially isomorphic, as easily follows from Part 2 of Lemma 9.2.

# 12 Back to graphs

#### 12.1 Proof of Theorem 1.2

Let G be a colored graph as defined in Section 2.1. Suppose that the color multiplicity of G is bounded by 4. By Theorem 2.5, G is amenable to 2-WL if and only if its coherent closure  $\mathcal{C}(G)$  is separable. Given G with n vertices, the coherent closure  $\mathcal{C}(G)$  is computable in time  $O(n^3 \log n)$  using the algorithm in [25]. Since G has color multiplicity at most 4, the coherent configuration  $\mathcal{C}(G)$  has only fibers with at most 4 points. Therefore, we can decide separability of  $\mathcal{C}(G)$  using the algorithm presented in Section 11. This algorithm reduces deciding separability for  $\mathcal{C}(G)$  to deciding separability for a number of irredundant subconfigurations  $\mathcal{C}_1, \ldots, \mathcal{C}_t$  such that

$$\bigcup_{i=1}^{t} F(\mathcal{C}_i) \subseteq F(\mathcal{C}(G)). \tag{53}$$

Producing the list of coherent configurations  $C_1, \ldots, C_t$  has low time complexity. For each  $i \leq t$ , we decide separability of  $C_i$  using the 2nd Approach presented in Section 10. Specifically,  $C_i$  is separable if and only if the associated vertex-colored graph  $G^i = G(C_i)$  is isomorphic to its modified version  $H^i = G^i_{X,C}$  for every  $X \in F(C_i)$ , where C is the hyperedge of  $D_{C_i}$  containing X. Here, G(C) refers to the construction of a graph from a given irredundant configuration described in Section 9; see Remark 10.2. Denote the number of vertices in  $G^i$  by  $n_i$ . The isomorphism algorithm for graphs of color multiplicity 4 in [1] performs a low-cost conversion of the pair  $(G^i, H^i)$  into a system of  $M_i < (n_i)^2$  linear equations with  $N_i < n_i$  unknowns over the field  $\mathbb{Z}_2$  such that  $G^i \cong H^i$  if and only if the system is consistent.

Specifically, we here describe a simplified version of this general reduction suitable for any pair  $(G^i, H^i)$  arising from  $\mathcal{C}_i$ . Recall that  $V(G^i) = V(H^i) = V(\mathcal{C}_i)$ , and the vertex color classes of both  $G^i$  and  $H^i$  are exactly the fibers  $X_1, \ldots, X_s$  of  $\mathcal{C}_i$ ,

where each  $X_j$  has the same color both in  $G^i$  and  $H^i$ . For every vertex color class  $X_j$ , we have  $G^i[X_j] = H^i[X_j]$ . Every non-empty bipartite subgraph  $G^i[X_j, X_k]$  is isomorphic to  $2K_{2,2}$ . In this case,  $H^i[X_j, X_k]$  is equal either to  $G^i[X_j, X_k]$  or to its bipartite complement.

Any isomorphism from  $G^i$  and  $H^i$  maps each vertex color class  $X_j$  onto itself. Moreover, if  $G^i$  and  $H^i$  are isomorphic, then there is an isomorphism  $\phi$  preserving each of the three matchings on  $X_j$  for every j (note that  $\phi$  is forced to preserve the matchings if  $\mathcal{C}_i[X_j]$  has at least two determined matchings and  $\phi$  can be modified to obey this condition if there is exactly one determined matching in  $\mathcal{C}_i[X_j]$ ). Denote the restriction of  $\phi$  to  $X_j$  by  $\phi_j$ . Thus,  $\phi_j$  is one of the four elements of the Klein group  $K(X_j)$ . Recall that a preserved matching can be either fixed or flipped. Denote the matchings on  $X_j$  by  $A_j, B_j, C_j$ . An element of  $K(X_j)$  is uniquely determined by a triple  $(a_j, b_j, c_j)$ , where  $a_j = 1$  if  $A_j$  is flipped and  $a_j = 0$  if  $A_j$  is fixed, and similarly for  $b_j$  and  $c_j$ . Since a non-identity element of K(X) fixes one matching and flips the other two, we have

$$(E_j) a_j \oplus b_j \oplus c_j = 0.$$

Another constraint on  $\phi_j$  is imposed by each pair  $X_j, X_k$  such that  $G^i[X_j, X_k]$  is non-empty. To be specific, suppose that  $C_i[X_j, X_k]$  determines the matching  $A_j$  in  $X_j$  and the matching  $B_k$  in  $X_k$ . Then

$$(E_{j,k}) a_j \oplus b_k = d_{j,k},$$

where  $d_{j,k} = 0$  if  $H^i[X_j, X_k]$  is equal to  $G^i[X_j, X_k]$  and  $d_{j,k} = 1$  if  $H^i[X_j, X_k]$  is the bipartite complement of  $G^i[X_j, X_k]$ . It remains to notice that a set of permutations  $\{\phi_j\}_{j=1}^s$  composing an isomorphism from  $G^i$  to  $H^i$  exists if and only if the system of equations consisting of  $(E_j)$  for all  $j \leq s$  and  $(E_{j,k})$  for all non-empty  $G^i[X_j, X_k]$  has a solution.

The rank of an  $M \times N$  matrix over a finite field is computable in time  $O(MN^{\omega-1})$ , where  $N \leq M$  (see [7, 23]), or in randomized time  $O(MN \log N + N^{\omega})$  (see [11]). Recall that we test isomorphism of  $|F(C_i)|$  pairs of graphs  $G^i$  and  $H^i$  and that, for each pair, our task is reduced to checking solvability of a linear system with  $3|F(C_i)|$  unknowns and at most  $\binom{|F(C_i)|}{2}$  equations. Since  $|F(C_i)| = n_i/4$ , in this way we can test separability of  $C_i$  in time  $O((n_i)^{2+\omega})$  deterministically or in time  $O((n_i)^4 \log n_i)$  using randomization. Taking into account the inequality  $\sum_{i=1}^t n_i \leq n$ , which follows from (53), and the general inequality

$$\sum_{i=1}^{t} (n_i)^{\alpha} \le \left(\sum_{i=1}^{t} n_i\right)^{\alpha}$$

for any real  $\alpha \geq 1$ , we conclude that separability of  $\mathcal{C}(G)$  is decidable in deterministic time  $O(n^{2+\omega})$  or in randomized time  $O(n^4 \log^2 n)$ , where an extra logarithmic factor corresponds to the number of repetitions needed to make the failure probability an arbitrarily small constant.

## 12.2 Small graphs

#### Theorem 12.1.

- 1. All graphs of color multiplicity 4 with at most 15 vertices are amenable.
- 2. Up to isomorphism and color renaming, there are 436 non-amenable graphs of color multiplicity 4 with 16 vertices. More precisely, the number of non-trivial ≡<sub>2-WL</sub>-equivalence classes is 218, each consisting of exactly two non-isomorphic graphs.
- *Proof.* 1. Let G be a graph of color multiplicity 4 with at most 15 vertices. By Theorem 2.5, G is amenable if and only if its coherent closure  $\mathcal{C}(G)$  is separable. Note that  $\mathcal{C}(G)$  has at most 15 points, and every fiber of  $\mathcal{C}(G)$  has size at most 4. By Part 1 of Theorem 11.1,  $\mathcal{C}(G)$  is separable.
- 2. Recall the notation introduced in Subsection 2.2 and the statement of Lemma 2.4. Given a colored graph G, let  $\mathcal{R}_G$  denote its underlying rainbow, that is, the partition of  $V(G)^2$  determined by the color classes of G. In particular, if G is a vertex-colored graph, then  $\mathcal{R}_G$  consists of the sets of loops vv of equally colored vertices, the set of pairs uv with adjacent u and v, and the set of pairs uv with non-adjacent u and v. The coherent closure  $\mathcal{C}(G) = \mathcal{C}(\mathcal{R}_G)$  is a refinement of the partition  $\mathcal{R}_G$ . Given a bijection  $f: \mathcal{C}(G) \to \mathcal{D}$  from  $\mathcal{C}(G)$  onto a rainbow  $\mathcal{D}$ , we extend f to a bijection from  $\mathcal{C}(G)^{\cup}$  onto  $\mathcal{D}^{\cup}$  by the rule  $(X_1 \cup \ldots \cup X_s)^f = X_1^f \cup \ldots \cup X_s^f$ . For each  $X \in \mathcal{R}_G$ , this defines its image  $X^f$  and, as usually, we have  $(\mathcal{R}_G)^f = \{X^f: X \in \mathcal{R}_G\}$ , which is a partition coarser than  $\mathcal{D}$ . Finally, we define  $G^f$  as the colored version of  $(\mathcal{R}_G)^f$  where each  $X^f$  inherits the color of the color class X of G. If G is a vertex-colored graph, then  $G^f$  is a vertex-colored graph as well.

We begin with stating a general fact that follows from Part 2 of Lemma 2.4 and the discussion preceding this lemma.

Claim B.  $G \equiv_{2\text{-WL}} H$  if and only if there is an algebraic isomorphism  $f : \mathcal{C}(G) \to \mathcal{C}(H)$  such that  $H = G^f$ .

According to Part 2 of Lemma 11.1, among all 16-point coherent configurations with maximum fiber size 4 there is a unique non-separable configuration  $\mathcal{T}$ . Moreover, the proof of this lemma shows that  $\mathcal{T}$  is the unique skew-connected configuration whose fiber graph  $F_{\mathcal{T}}$  is isomorphic to the complete graph  $K_4$ . Let G be a vertex-colored graph of color multiplicity 4 on 16 vertices. By Theorem 2.5, G is non-amenable if and only if  $\mathcal{C}(G) \cong_{comb} \mathcal{T}$ . Looking for non-amenable graphs, we can therefore assume that  $\mathcal{C}(G) = \mathcal{T}$ .

Combining Claim B with Lemma 7.1, we conclude that  $G \equiv_{2\text{-WL}} H$  if and only if there is a strict algebraic automorphism f of  $\mathcal{T}$  such that  $H \cong G^f$ . Looking for graphs H such that  $G \equiv_{2\text{-WL}} H$ , we can therefore assume that  $H = G^f$  for  $f \in \mathbb{A}(\mathcal{T})$ . If  $f \in \mathbb{A}^*(\mathcal{T})$ , i.e., f is induced by a combinatorial automorphism  $\phi$  of  $\mathcal{T}$ , then obviously  $\phi$  is an isomorphism from G to H. Conversely, if  $G \cong H$ , then

 $f \in \mathbb{A}^*(\mathcal{T})$  by Part 3 of Lemma 2.4. Thus,

$$G \equiv_{2\text{-WL}} G^f \text{ and } G \ncong G^f \text{ iff } f \in \mathbb{A}(\mathcal{T}) \setminus \mathbb{A}^*(\mathcal{T}).$$
 (54)

Note that the difference  $\mathbb{A}(\mathcal{T}) \setminus \mathbb{A}^*(\mathcal{T})$  is non-empty by Part 3 of Lemma 8.1 because  $\mathcal{T}$  is skew-connected and  $\delta(F_{\mathcal{T}}) = 3$ . We now generalize the equivalence (54) as follows.

Claim C. Suppose that  $C(G) = \mathcal{T}$ . Let  $h, f \in \mathbb{A}(\mathcal{T})$ . Then  $G^h \cong G^f$  if and only if  $h^{-1}f \in \mathbb{A}^*(\mathcal{T})$ .

Proof of Claim C. Denote  $A = G^h$  and note that  $G^f = A^{h^{-1}f}$ . We obtain the claim by applying the equivalence (54) to A.  $\triangleleft$ 

Consider  $h, f \in \mathbb{A}(\mathcal{T}) \setminus \mathbb{A}^*(\mathcal{T})$ . By Part 3 of Lemma 8.1,  $\mathbb{A}^*(\mathcal{T})$  is a subgroup of  $\mathbb{A}(\mathcal{T})$  of index 2. This implies that  $h^{-1}f \in \mathbb{A}^*(\mathcal{T})$  and, hence,  $G^h \cong G^f$  by Claim C. It follows that, if each of two graphs  $H_1$  and  $H_2$  is  $\equiv_{2\text{-WL}}$ -equivalent but not isomorphic to G, then  $H_1$  and  $H_2$  are isomorphic to each other. This proves that every non-trivial  $\equiv_{2\text{-WL}}$ -equivalence class of 16-vertex graphs of color multiplicity 4 contains exactly two graphs. It remains to count the number of such classes.

We first describe the structure of graphs G of color multiplicity 4 with  $\mathcal{C}(G) = \mathcal{T}$ . Clearly, any such G has 4 vertex color classes, each consisting of 4 vertices. More precisely, the vertex color classes of G are exactly the fibers of  $\mathcal{T}$ . For any two fibers X and Y, the interspace  $\mathcal{T}[X,Y]$  is a refinement of the partition of  $X \times Y$  accordingly to the adjacency relation of G[X,Y]. It follows that G[X,Y] is isomorphic either to  $2K_{2,2}$  or to  $K_{4,4}$ . The latter option is actually impossible. Indeed, assume that  $G[X,Y] \cong K_{4,4}$  and let  $\mathcal{T}_-$  be obtained from  $\mathcal{T}$  by making the interspace  $\mathcal{T}[X,Y]$  uniform. Note that

$$\mathcal{T} \prec \mathcal{T}_{-} \preccurlyeq \mathcal{R}_{G}$$

and that  $\mathcal{T}_{-}$  is a coherent configuration (because every subconfiguration  $\mathcal{T}_{-}[A \cup B \cup C]$  for  $A, B, C \in F(\mathcal{T}_{-})$  is obviously coherent). This contradicts Proposition 2.1.

Furthermore, the induced subgraph G[X] for each vertex color class X must be regular, that is, G[X] is either empty or isomorphic to  $K_4$ ,  $C_4$ , or  $2K_2$ . We conclude that every 16-vertex G of color multiplicity 4 with  $\mathcal{C}(G) = \mathcal{T}$  is one of the graphs obtainable in the following way:

- Step 1. Take four disjoint 4-vertex sets  $X_1, X_2, X_3, X_4$  and color them in four colors so that each  $X_i$  is monochromatic.
- Step 2. For each two indices i and j, connect  $X_i$  and  $X_j$  with 8 edges so that  $G[X_i, X_j] \cong 2K_{2,2}$ . Note that  $G[X_i, X_j]$  determines a matching on  $X_i$  and a matching on  $X_j$ . It is required that, for every i, the three subgraphs  $G[X_i, X_j]$  for  $j \in \{1, 2, 3, 4\} \setminus \{i\}$  determine three pairwise distinct matchings on  $X_i$ .
- Step 3. For each i, either leave  $G[X_i]$  empty or plant a  $K_4$ -, or  $C_4$ -, or  $2K_2$ -subgraph on  $X_i$ .

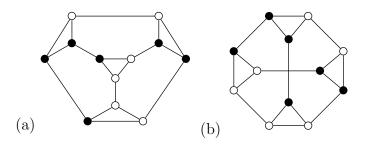


Figure 18: A colored truncated tetrahedral graph (two looks).

We claim that  $C(G) \cong \mathcal{T}$  for every graph G obtainable as described above. Due to Step 2, the edges of G between the classes  $X_1, X_2, X_3, X_4$  represent a coherent configuration  $\mathcal{T}$  with fibers  $X_1, X_2, X_3, X_4$ . Since any  $K_4$ -,  $C_4$ -, or  $2K_2$ -subgraph planted in Step 3 can be split into matching, we have

$$\mathcal{T} \preccurlyeq \mathcal{R}_G.$$
 (55)

On the other hand, note that the vertex coloring of G determines the partition of the diagonal  $\{vv: v \in V(G)\}$  into four reflexive relations, each of size 4, corresponding to the fibers of  $\mathcal{T}$ . Each  $G[X_i, X_j]$  determines the partition of  $X_i \times X_j$  of  $2K_{2,2}$ -type corresponding to the interspace  $\mathcal{T}[X_i, X_j]$ . Moreover, each  $G[X_i, X_j]$  determines a matching on  $X_i$  in the sense of Part 2 of Lemma 5.2. Due to Step 2, this determines the  $F_4$ -factorization of each  $(X_i)^2$ . In terms of partitions, these observations can be stated as

$$C(G) \preccurlyeq T. \tag{56}$$

Relations (55) and (56) imply by Proposition 2.1 that C(G) = T.

Thus, we have described the family of all G of color multiplicity 4 with  $\mathcal{C}(G) \cong \mathcal{T}$ . However, following Steps 1–3, we can generate the same, up to isomorphism, graph in many different ways. Now, we want to count the number of such graphs up to isomorphism and color renaming. As we already know that every non-trivial  $\equiv_{2\text{-WL}}$ -equivalence class consists of two non-isomorphic graphs, we can count the number of these classes and multiply it by 2.

Suppose that G is obtained according to Steps 1–3. With G we associate a truncated tetrahedral graph  $T_G$  whose vertices are colored black or white; see Figure 18(a). Denote the three matchings on the vertex color class  $X_i$  of G by  $L_i$ ,  $M_i$ , and  $N_i$ . The vertex set of  $T_G$  is  $\{L_i, M_i, N_i\}_{i=1}^4$ . Each triple  $\{L_i, M_i, N_i\}$  forms a 3-clique. Moreover, a vertex  $M \in \{L_i, M_i, N_i\}$  is adjacent to a vertex  $M' \in \{L_j, M_j, N_j\}$  whenever  $G[X_i, X_j]$  determines M on  $X_i$  and M' on  $X_j$ . The edge set of  $T_G$  is therewith defined. A vertex  $M \in \{L_i, M_i, N_i\}$  is colored black if M is covered by the adjacency relation of  $G[X_i]$  and it is colored white otherwise. Thus, the clique  $\{L_i, M_i, N_i\}$  contains 3, 2, 1 black vertices exactly when  $G[X_i]$  is isomorphic to  $K_4$ ,  $C_4$ ,  $2K_2$  respectively. All vertices in  $\{L_i, M_i, N_i\}$  are white exactly when  $X_i$  is an independent set in G.

Claim D. G and H are  $\equiv_{2\text{-WL}}$ -equivalent up to color renaming if and only if  $T_G \cong T_H$ .

Proof of Claim D. Denote C = C(G) and D = C(H). Note that  $T_G$  does not change after renaming the colors in G. To prove the claim in the forward direction, we can therefore assume that  $G \equiv_{2\text{-WL}} H$ . By Claim B, there is an algebraic isomorphism  $f: C \to D$  such that  $H = G^f$ . Each of the matching relations  $L_i$ ,  $M_i$ , and  $N_i$  is in C and, therefore, the restriction of f to the matching relations can be seen as a bijection from  $V(T_G)$  onto  $V(T_H)$ . Since the algebraic isomorphism f takes the fibers of C to the fibers of D, f takes the 3-cliques of  $T_G$  to the 3-cliques of  $T_H$ . Since f preserves the relation "an interspace f determines a matching f takes the remaining edges of f to the remaining edges of f provides an isomorphism from f to f. Therefore, f provides an isomorphism from f to f.

Assume now that  $T_G \cong T_H$ . Given an isomorphism  $\alpha$  from  $T_G$  to  $T_H$ , we construct an algebraic isomorphism  $f: \mathcal{C} \to \mathcal{D}$  such that  $H = G^f$ , possibly after appropriately renaming the colors of vertices in H. By Claim B, this will imply that  $G \equiv_{2\text{-WL}} H$  up to color renaming.

We first define f on the set of the matching relations in C just by setting f(M) = $\alpha(M)$  for each of the 12 matchings. The isomorphism  $\alpha$  takes the 3-cliques of  $T_G$ to the 3-cliques of  $T_H$ . Therefore, if M and M' are matchings on the same fiber of  $\mathcal{C}$ , then f(M) and f(M') are matchings on the same fiber of  $\mathcal{D}$ . Using this, we can consistently extend f to a bijection from the set of the reflexive relations of C to the reflexive relations of  $\mathcal{D}$ . For a fiber  $X_i$  of  $\mathcal{C}$ , we will denote the corresponding fiber of  $\mathcal{D}$  by  $f(X_i)$ . Renaming the vertex colors in H if necessary, we can ensure that the vertex color classes  $X_i$  in G and  $f(X_i)$  in H are equally colored. Finally, for each pair of fibers  $X_i, X_j \in F(\mathcal{C})$ , we define f locally as a bijection from the interspace  $\mathcal{C}[X_i, X_j]$  onto the interspace  $\mathcal{D}[f(X_i), f(X_j)]$  in the following way: The element of  $\mathcal{C}[X_i, X_i]$  corresponding to the adjacency relation of  $G[X_i, X_i]$  is taken by f to the element of  $\mathcal{D}[f(X_i), f(X_i)]$  corresponding to the adjacency relation of  $H[f(X_i), f(X_i)]$ . Thus, we have defined a bijection f from  $\mathcal{C}$  onto  $\mathcal{D}$ . Since  $\alpha$ preserves adjacency between vertices in different 3-cliques, f preserves the relation "an interspace I determines a matching M". This implies that f is an algebraic isomorphism from  $\mathcal{C}$  onto  $\mathcal{D}$ .

It remains to argue that  $H = G^f$ . Suppose that a relation  $R \in \mathcal{C}$  is covered by the adjacency relation of G. We have to verify that the relation  $R^f \in \mathcal{D}$  is covered by the adjacency relation of H. If R belongs to an interspace of  $\mathcal{C}$ , this follows directly from the definition of f. If R belongs to a cell of  $\mathcal{C}$ , that is, is a matching relation, this follows from the fact that  $\alpha$  preserves the black-white vertex coloring. It remains to note that the correspondence between the reflexive color relations in G and H was secured by color renaming.  $\triangleleft$ 

Claim D reduces our task to counting the non-isomorphic black-white colorings of the truncated tetrahedral graph T. We use the Pólya enumeration theorem. Let  $\operatorname{Aut}(T)$  be the subgroup of the symmetric group  $S_{12}$  consisting of the automorphisms of T. Every automorphism of T takes a 3-clique to a 3-clique, determining a permutation of the 4-element set of all 3-cliques. This actually yields a one-to-one

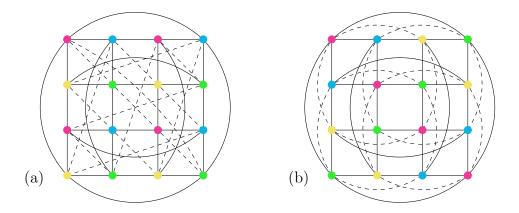


Figure 19: An example of 2-WL-equivalent non-isomorphic colored graphs: (a) The Shrikhande graph; (b) the  $4 \times 4$  rook's graph.

correspondence between  $\operatorname{Aut}(T)$  and  $S_4$  in accordance with the fact that the regular tetrahedron has the same isometries as its truncated version. As a consequence, the permutations in  $\operatorname{Aut}(T)$ , like in  $S_4$ , are split into 5 conjugacy classes. One class consists of the identity permutation, which in  $\operatorname{Aut}(T)$  has 12 cycles. The six transpositions in  $S_4$  correspond to reflections in a plane, which for the truncated tetrahedron give six permutations with 7 cycles each, seen in Figure 18(a) as reflections in a line. The eight 3-cycles in  $S_4$  correspond to axial rotations, which for the truncated tetrahedron give eight permutations with 4 cycles each, seen as rotations in Figure 18(a). The six 4-cycles in  $S_4$  correspond to six permutations in  $\operatorname{Aut}(T)$  with 3 cycles each, which can be seen as rotations in Figure 18(b). Finally, three products of two transpositions in  $S_4$  correspond to three permutations in  $\operatorname{Aut}(T)$  with 6 cycles each, which appear in Figure 18(b) as the inversion in the central point. By the Pólya enumeration theorem, the number of non-isomorphic ways to color the vertices of T in n colors is equal to

$$p(n) = \frac{1}{24} \left( n^{12} + 6 n^7 + 3 n^6 + 8 n^4 + 6 n^3 \right).$$

The number of different colorings in two colors is, therefore, equal to p(2) = 218.  $\square$ 

To illustrate Part 2 of Theorem 12.1, we show two  $\equiv_{2\text{-WL}}$ -equivalent and still non-isomorphic graphs produced as in the proof, with all color classes left empty in Step 3. Remarkably, these are colored versions of two smallest non-isomorphic strongly regular graphs with the same parameters, namely the Shrikhande graph and the  $4 \times 4$  rook's graph both having parameters (16,6,2,2); see Figure 19(a)–(b).

# 13 Further questions

Our results raise questions about the parameterized complexity of recognizing amenability of a given graph with the color multiplicity m taken as the parameter. The problem is trivial for m=3 due to [25]. We show that it is solvable in polynomial time for m=4. Our analysis surely generalizes to a few subsequent values of m. For any fixed m, the problem is in coNP, and it is open whether it is in P if m is large.

Another open question, that naturally arises in light of Theorem 1.2, concerns the next dimension of the Weisfeiler-Leman algorithm: Can the amenability to 3-WL be decided in polynomial time on input graphs of color multiplicity 4?

The WL dimension of a graph G is defined as the minimum k such that G is amenable to k-WL. The graphs with large WL dimension are of significant interest in the study of the graph isomorphism problem. When we seek such graphs among graphs with color multiplicity 4, note that they must be at least non-amenable to 2-WL. Cai, Fürer, and Immerman [9] give conditions ensuring linear WL dimension for graphs whose coherent closure is, in our terminology, skew-connected. Further such conditions are identified by the line of research [12, 20, 32, 33]. Can we achieve high WL dimension in other cases, say, for graphs whose coherent closure corresponds to a line-point  $(n_3)$ -configuration?

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